WEST Search History

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DATE: Wednesday, June 21, 2006

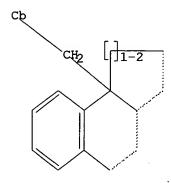
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STRUCTURE UPLOADED

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Structure attributes must be viewed using STN Express query preparation.

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8 SEA SSS SAM L1

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L489 L3

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(PD<19990400)

L5 40 L4 AND PD< APRIL 1999

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L5ANSWER 1 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN1999:812631 CAPLUS

DN 132:165996

Mechanochemical arylation and alkylation of fullerene C60 under the solvent-free conditions

AU Tanaka, Toru; Komatsu, Koichi

CS Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan

SO Synthetic Communications (1999), 29(24), 4397-4402 CODEN: SYNCAV; ISSN: 0039-7911

Marcel Dekker, Inc. PB

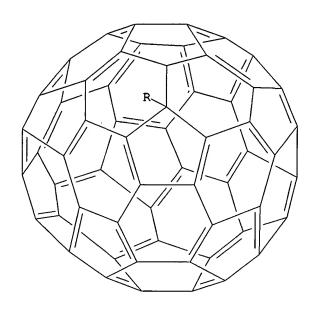
Journal DT

- LA English
- OS CASREACT 132:165996
- AB The mechanochem. reaction of fullerene C60 with organic bromides and alkali metals gave the corresponding aryl or alkyl C60 derivs. under the solvent-free conditions.
- IT 170646-75-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (mechanochem. arylation and alkylation of fullerene C60 under solvent-free conditions)

- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)





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RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 2 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1999:735295 CAPLUS
- DN 132:137266
- TI Tandem nucleophilic addition/Diels Alder reaction of N-butadienyl N,O-Ketene silyl acetals with C60: stereoselective formation of bicyclic octahydroquinolino-1,2,3,4-tetrahydrobuckminsterfullerenes and combined NMR spectroscopic and computational evaluation of the functionalization reactions
- AU Rubin, Yves; Ganapathi, Padma S.; Franz, Andreas; An, Yi-Zhong; Qian, Wenyuan; Neier, Reinhard
- CS Department of Chemistry and Biochemistry, University of California. Los Angeles, Los Angeles, CA, 90095-1569, USA

- SO Chemistry--A European Journal (1999), 5(11), 3162-3184 CODEN: CEUJED; ISSN: 0947-6539
- PB Wiley-VCH Verlag GmbH
- DT Journal
- LA English
- OS CASREACT 132:137266
- We have studied the reactivity of N,O-ketene N-1,3-butadienyl-N-alkyl-Osilyl acetals (Z)-RCH:CH(OSiMe2CMe3)N(R1)CH:CHCH:CH2 (R = Me2CH, PhCH2, 9-anthracenylmethyl, 4-MeOC6H4CH2; R1 = Me, 4-MeOC6H4, H2C:CH) (I) with C60 proceeding through a tandem process to give tricyclic octahydroquinolinyl fullerene adducts. Deprotonation of the tricyclic octahydroquinolinyl fullerene adducts with sodium hydride and addition of alkylating agents such as Me iodide, allyl bromide, or benzyl bromide yield adducts alkylated on the fullerene. The addition order of these tandem reactions has been evaluated. The initial nucleophilic Michael-like addition of I proceeds unusually fast at 25°C, followed by an intramolecularly accelerated Diels - Alder step that is highly diastereoselective. The structures of the tricyclic octahydroquinolinyl fullerene adducts were determined from the 1H and 13C NMR shifts and from H - H coupling patterns, while their stereochem. was deduced from 2D T-ROESY NMR expts. The proposed mechanism for the nucleophilic addition involves single electron transfer followed by radical anion - radical cation recombination. Computational investigations of the reaction pathways, transition states, and conformational energies have been carried out to corroborate the exptl. data.

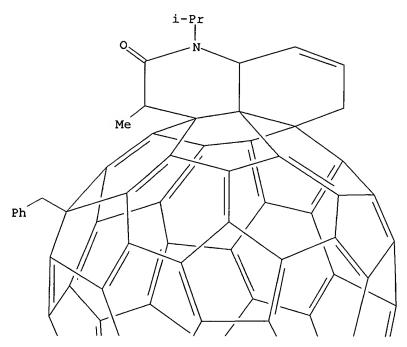
IT 256652-27-4P

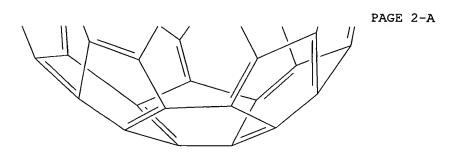
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of fullerene derivs. by deprotonation of octahydroquinolinyl fullerenes and addition of electrophiles)

RN 256652-27-4 CAPLUS

CN 1'H,14H-[5,6]Fullereno-C60-Ih-[2,1,9-de]quinolin-2'(3'H)-one, 6',8'a-dihydro-3'-methyl-1'-(1-methylethyl)-14-(phenylmethyl)-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A





RE.CNT 157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

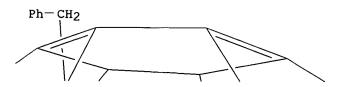
- L5 ANSWER 3 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1999:654258 CAPLUS
- DN 131:315178
- TI Electrosynthesis and characterization of (C6H5CH2)4C60 isomers
- AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Proceedings Electrochemical Society (1999), 99-12(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 92-114
 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society

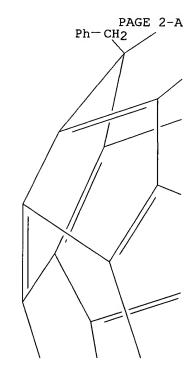
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DT
     Journal
LΑ
     English
AB
     The structural, spectral, and electrochem. properties of 2 (C6H5CH2)4C60
     isomers are reported. One is designated as the 1,4,1,4-(C6H5CH2)4C60
     isomer and the other as the 1,4,1,2-isomer of (C6H5CH2)4C60.
     1,4,1,2-isomer is the first example of an organofullerene possessing both
     1,4- and 1,2-addition patterns. The 2 isomers were isolated by HPLC from the
     products produced in a reaction between the diamion of (C6H5CH2)2C60 and
     C6H5CH2Br. X-ray data show that the 2 organofullerenes differ from one
     another by the position of only 1 benzyl group with the 4 benzyl
     substituents being in close proximity to each other in each compound Both
     (C6H5CH2)\,4C60 isomers undergo 3 one-electron redns. in PhCN containing 0.1 M
     tetra-n-butylammonium perchlorate (TBAP) and have E1/2 values which are
     more neg. than those of either C60 or 1,4-(C6H5CH2)2C60. The monoanions
     of 1,4,1,4- and 1,4,1,2-(C6H5CH2)4C60 were electrogenerated by bulk
     controlled-potential electrolysis in PhCN containing 0.2 M TBAP and
     characterized as to their spectral properties in both the visible and near
     IR regions.
IT
     207684-63-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (in electrosynthesis of (C6H5CH2)4C60 isomers)
RN
     207684-63-7 CAPLUS
CN
     [5,6]Fullerene-C60-Ih, 1,2,3,13-tetrahydro-3,13-bis(phenylmethyl)-,
     ion(2-) (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
ΙT
     247185-05-3 247185-06-4
     RL: PRP (Properties)
        (spectral data of monoanions of (C6H5CH2)4C60 isomers prepared by
        electrosynthesis)
RN
     247185-05-3 CAPLUS
CN
     [5,6]Fullerene-C60-Ih, 1,6,11,18-tetrahydro-1,6,11,18-
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tetrakis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)

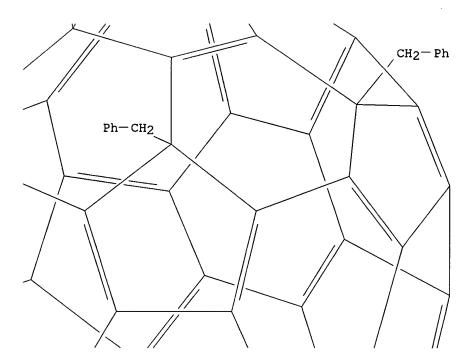
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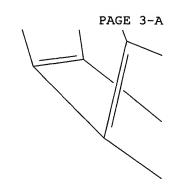
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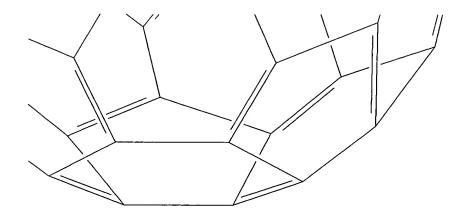




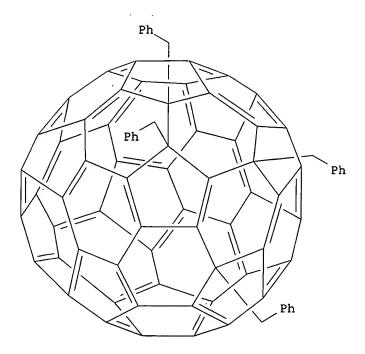




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RN 247185-06-4 CAPLUS
CN [5,6]Fullerene-C60-Ih, 1,6,9,18-tetrahydro-1,6,9,18-tetrakis(phenylmethyl), radical ion(1-) (9CI) (CA INDEX NAME)



IT 207684-64-8P 247185-87-1P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (structural, spectral, and electrochem. properties of (C6H5CH2)4C60 isomers)

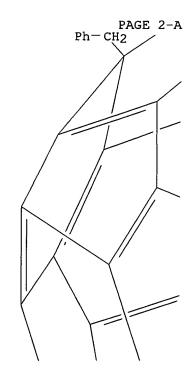
RN 207684-64-8 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,6,11,18-tetrahydro-1,6,11,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

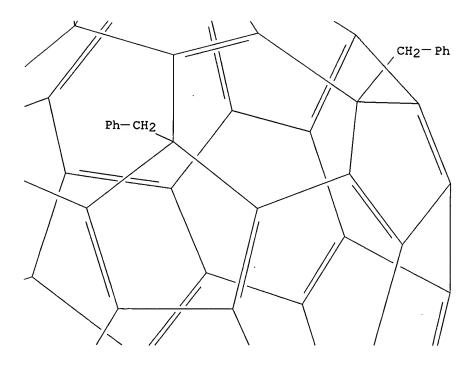
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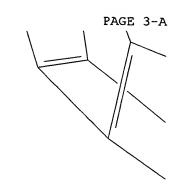
PAGE 1-B



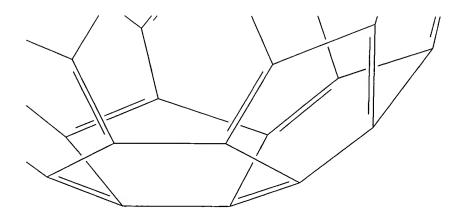




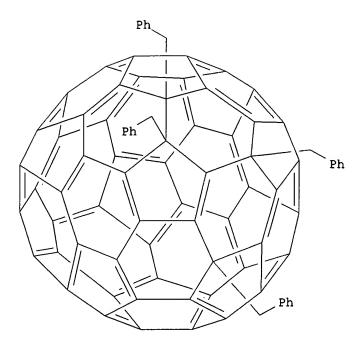




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RN 247185-87-1 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,6,9,18-tetrahydro-1,6,9,18-tetrakis(phenylmethyl)-(9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 4 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1999:560721 CAPLUS
- DN 131:350971
- TI Radical functionalization of [60] fullerene and its derivatives initiated by the C(CF3)2C6H4F radical
- AU Tumanskii, B. L.; Kalina, O. G.; Bashilov, V. V.; Usatov, A. V.; Shilova, E. A.; Lyakhovetskii, Yu. I.; Solodovnikov, S. P.; Bubnov, N. N.; Novikov, Yu. N.; Lobach, A. S.; Sokolov, V. I.
- CS A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 117813, Russia
- SO Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1999), 48(6), 1108-1112 CODEN: RCBUEY; ISSN: 1066-5285
- PB Consultants Bureau
- DT Journal
- LA English
- AB It was found that the 2-(p-fluorophenyl)hexafluoroisopropyl radical produced by thermal dissociation of the Polishchuk dimer [C(CF3)2C6H4F]2 can withdraw, under mild conditions, the H atom from the Me group of toluene and mesitylene to form the corresponding radicals, whose addition to [60]fullerene occurs more selectively than in the case of photochem. production of these radicals. Dynamics of the step-by-step multiaddn. of the radicals to C60 was studied by ESR. It was found that the addition of benzyl radicals affords adducts containing from 3 to 5 benzyl groups, whereas no spin-adducts with five addends were observed for more bulky 3,5-dimethylphenylmethyl radicals. The interaction of 3,5-dimethylphenylmethyl radicals with the metal complexes (η2-C60)[IrH(CO)(PPh3)2] and (η2-C60)[Pd(PPh3)2] was studied for the first time. It was shown that the palladium derivative undergoes only demetalation. In the case of the Ir complex, up to 3 radicals add to the

fullerene ligand in the same hemisphere where the transition metal is coordinated. The reaction rates are .apprx.5 times lower than those for C60. The ability of 2-(p-fluorophenyl) hexafluoroisopropyl radicals to dehydrogenate C60H36 was found.

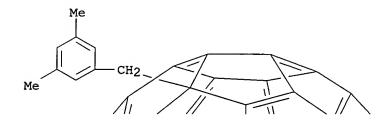
IT 245476-77-1

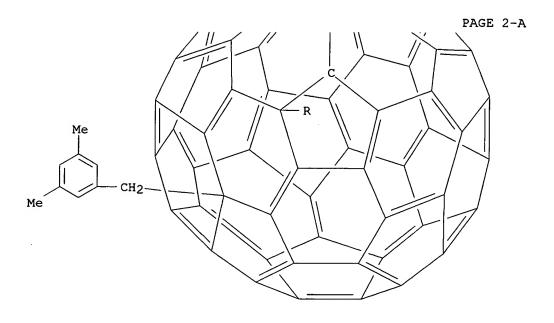
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (radical functionalization of [60] fullerene and its organometallic derivs. initiated by the C(CF3) 2C6H4F-p radical)

RN 245476-77-1 CAPLUS

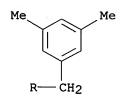
CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2,10,14-tris[(3,5-dimethylphenyl)methyl]-10,14-dihydro- (9CI) (CA INDEX NAME)

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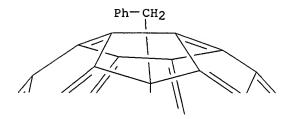
IT 139141-78-9 140700-29-4 250671-55-7

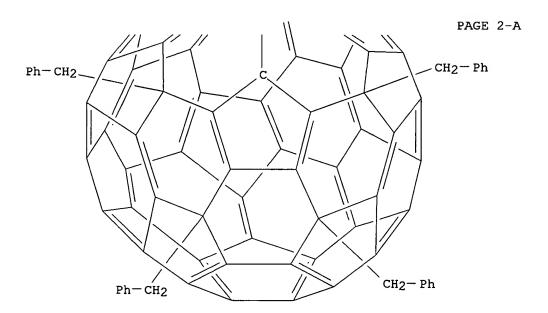
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (radical functionalization of [60] fullerene and its organometallic

derivs. initiated by the C(CF3)2C6H4F-p radical) 139141-78-9 CAPLUS

RN

CN [5,6]Fulleren-C60-Ih-1(9H)-yl, 6,12,15,18-tetrahydro-6,9,12,15,18-pentakis(phenylmethyl)- (9CI) (CA INDEX NAME)





RN 140700-29-4 CAPLUS CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-(9CI) (CA INDEX NAME) *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 250671-55-7 CAPLUS

CN Iridium, carbonyl[(3,15-\eta)-10,14-dihydro-2,10,14-tris[(3,5-dimethylphenyl)methyl][5,6]fulleren-C60-Ih-1(2H)-yl]hydrobis(triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)

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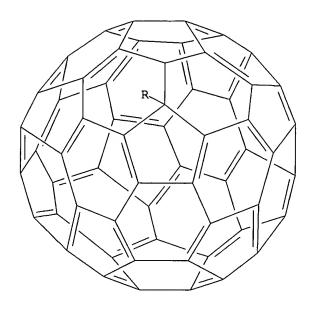
PAGE 3-A

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RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 5 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1999:392433 CAPLUS
- DN 131:129618
- TI [60] Fullerene radical cation: reactions and mechanism
- AU Siedschlag, Christina; Luftmann, Heinrich; Wolff, Christian; Mattay, Jochen
- CS Institut Organische Chemie, Christian-Albrechts-Universitat Kiel, Kiel, D-24098, Germany
- SO Tetrahedron (1999), 55(25), 7805-7818 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- AB C60 was irradiated in the presence of several electron transfer photosensitizers. Upon addition of H-donors such as N,N-dimethylformamide, 1,3-dioxolane, phenylacetaldehyde, Me formate, tert-butanol, propionic acid, glycol and methoxyethanol, 1-substituted 1,2-dihydro[60]fullerenes and in one case a 1,2,3,4-tetrahydro[60]fullerene were formed. A mechanistic pathway involving C60+ is proposed.
- IT 170646-75-0P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (mechanism of photoinduced electron transfer mediated addition of hydrogen donors to C60 fullerene)
- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

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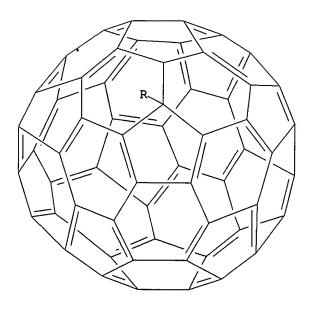
CH2-Ph

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 6 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1999:251966 CAPLUS
- DN 131:37660
- TI Radical ions in fullerene chemistry
- AU Siedschlag, Ch.; Torres-Garcia, G.; Wolff, Ch.; Mattay, J.; Fujitsuka, M.; Watanabe, A.; Ito, O.; Dunsch, L.; Ziegs, F.; Luftmann, H.
- CS Institut fur Organische Chemie, Universitat Kiel, Kiel, D-24098, Germany
- SO Journal of Information Recording (1998), 24(3-4), 265-270 CODEN: JIREFL; ISSN: 1025-6008
- PB Gordon & Breach Science Publishers
- DT Journal
- LA English
- AB [60]Fullerene is irradiated in the presence of several electron transfer photosensitizers. Upon addition of various H-donors 1-substituted 1,2-dihydro-[60]fullerenes are formed. Mechanistic studies using laser flash photolysis as well as ESR spectroscopy reveal the formation of the radical cation of [60]fullerene. In addition the [2 + 2]photoreactions of 4-methyl-1,2,4-triazoline-3,5-dione with [60]fullerene derivs. are reported.
- IT 170646-75-0P
 - RL: PNU (Preparation, unclassified); PREP (Preparation) (formation from fullerene by photolysis in presence of hydrogen donor and electron transfer photosensitizer)
- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX

NAME)

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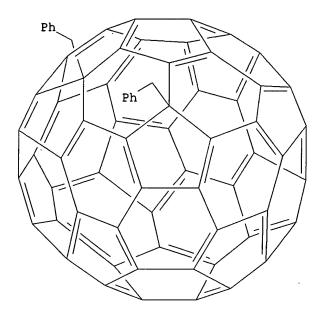


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 7 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:638828 CAPLUS
- DN 129:330532
- TI Alkylation of C602- generated from C60H2
- AU Meier, Mark S.; Bergosh, Robert G.
- CS Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA
- SO Proceedings Electrochemical Society (1998), 98-8(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 1103-1109
 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- AB The preparation of mono- and dialkylfullerenes from C60H2 is reported. Deprotonation of C60H2 with tetrabutylammonium hydroxide in benzonitrile generates C602- dianion, which reacts rapidly with selected alkyl halides. Alkylation is successful when the alkylating agent can generate relatively stable radicals. Tosylates are unreactive in both the first and second alkylation step. The monoalkylated fullerenes were obtained as 1,2-regioisomers, while dialkylfullerenes were obtained as 1,4 regioisomers.
- IT 176106-61-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(selective mono- and dialkylation of C602- generated from C60H2)
176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 8 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:569500 CAPLUS
- DN 129:244749

RN

- TI Formation of C60 Adducts with Two Different Alkyl Groups via Combination of Electron Transfer and SN2 Reactions
- AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, Takeomi; Arakawa, Ryuichi; Kadish, Karl M.
- CS Department of Material and Life Science Graduate School of Engineering, Osaka University, Suita Osaka, 565-0871, Japan
- SO Journal of the American Chemical Society (1998), 120(36), 9220-9227
 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 129:244749
- AB The formation of organofullerenes of the type R2C60 and R(R')C60 from C602- and alkyl halides (RX or R'X) in benzonitrile was mechanistically investigated for 15 different alkyl halides which vary in electrophilicity and electron acceptor ability. The first step in the reaction leads to RC60- via an electron-transfer mechanism, followed by formation of R2C60 or R(R')C60 via an SN2 mechanism. Evidence of the mechanism comes from comparison of rate consts. for the stepwise addition of two R groups to C602-with rate consts. for the genuine electron transfer and SN2 reactions. The formation of t-BuC60- and PhCH2C60- after the first R group addition was confirmed by electrospray ionization mass spectroscopy. The t-BuC60-

derivative will not react further with excess t-BuI, but this is not the case for the less sterically hindered PhCH2Br, which adds to t-BuC60- in benzonitrile to give t-Bu(PhCH2)C60. A protonation of t-BuC60- with trifluoroacetic acid can also occur to give 1,4-t-Bu(H)C60, which rearranges rapidly to yield 1,2-t-Bu(H)C60. Rate consts. for the second alkylation of t-BuC60- with a variety of different alkyl halides are compared with values of genuine SN2 reactions and indicate that the second step in the fullerene alkylation reaction proceeds via an SN2 mechanism. The rate consts. of electron transfer from C602- to RX span a range of 105, but are insensitive to the steric effect of the alkyl group, i.e., they depend only on the electron-acceptor ability of RX. In contrast, the SN2 rate consts. of t-BuC60- with RX are highly susceptible to the steric effect of the alkyl group and no reaction at all takes place between t-BuC60- and t-BuI. Thus, the first addition of one sterically hindered alkyl group to C602- occurs via electron transfer and cannot be followed by further addition of a second sterically hindered group (via an SN2 reaction). This is not the case for less sterically hindered alkyl groups such as benzyl bromide which can add via an SN2 reaction to yield C60 adducts with two different alkyl groups.

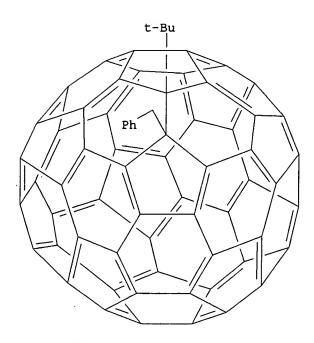
IT 195392-52-0

RL: PRP (Properties)

(calculated formation enthalpy; formation of C60 adducts with two different alkyl groups via combination of electron transfer and SN2 reactions)

RN 195392-52-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,9-dihydro-9-(phenylmethyl)-(9CI) (CA INDEX NAME)



IT 182070-59-3

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation of C60 adducts with two different alkyl groups via combination of electron transfer and SN2 reactions)

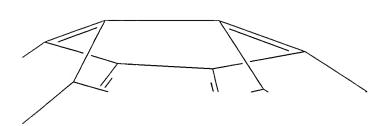
RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA

INDEX NAME)

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10/721,318 (RCE)

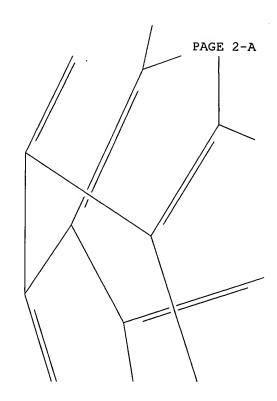
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * IT 160482-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(formation of C60 adducts with two different alkyl groups via
combination of electron transfer and SN2 reactions)

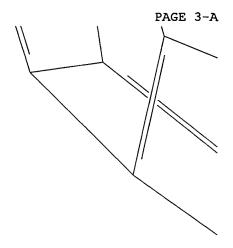
RN 160482-48-4 CAPLUS

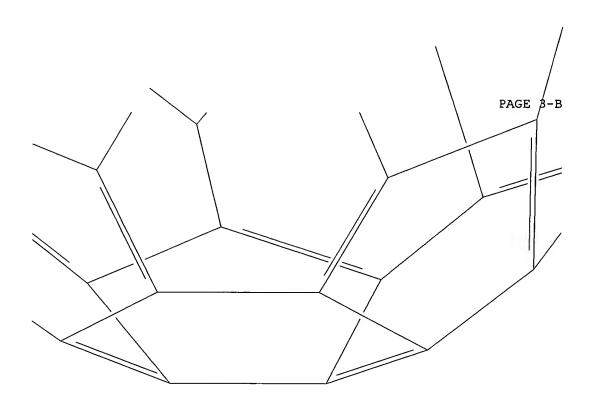
- CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-(9CI) (CA INDEX NAME)
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 1-C



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *







RE.CNT 136 THERE ARE 136 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 9 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:499423 CAPLUS
- DN 129:195665
- TI Selective One-Electron and Two-Electron Reduction of C60 with NADH and NAD Dimer Analogs via Photoinduced Electron Transfer
- AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Patz, Matthias; Hirasaka, Takeomi; Itoh, Shinobu; Fujitsuka, Mamoru; Ito, Osamu
- CS Department of Material and Life Science Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan
- SO Journal of the American Chemical Society (1998), 120(32), 8060-8068
 - CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society

- DT Journal
- LA English
- AB The selective one-electron reduction of C60 to C60•- is attained through photoinduced electron transfer from an NADH analog, 1-benzyl-1,4dihydronicotinamide (BNAH), and the dimer analog [(BNA)2] to the triplet excited state of C60. The limiting quantum yield for formation of C60-- in the case of (BNA)2 exceeds unity; $\Phi_{\infty} = 1.3$. In this case, the initial electron transfer from (BNA)2 to the triplet excited state (3C60*) is followed by fast C-C bond cleavage in the resulting (BNA) 2++ to give BNA+ and BNA+ and the second electron transfer from BNA• to C60 yields BNA+ and C60•-, when (BNA)2 acts as a two-electron donor to produce 2 equiv of C60 -. When BNAH is replaced by 4-tert-butylated BNAH (t-BuBNAH), the photochem. reaction with C60 yields not C60 - but instead the tert-butylated anion (t-BuC60-) selectively. In this case, the initial electron transfer from t-BuBNAH to 3C60* is also followed by fast C-C bond cleavage in t-BuBNAH•+ to give t-Bu•, which is coupled with C60•- produced in the electron transfer to yield t-BuC60-. The selective two-electron reduction of C60 to 1,2-dihydro[60] fullerene (1,2-C60H2) is also attained with the use of another NADH analog, 10-methyl-9,10-dihydroacridine (AcrH2), under visible light irradiation in deaerated benzonitrile solution containing trifluoroacetic acid.

The studies on the quantum yields, the kinetic deuterium isotope effects, and the quenching of the triplet-triplet absorption of C60 by AcrH2 have revealed that the photochem. reduction proceeds via photoinduced electron transfer from 10-methyl-9,10-dihydroacridine to the triplet excited state of C60, which is followed by proton transfer from AcrH2+ to C60-and a second electron transfer from the deprotonated acridinyl radical (AcrH+) to C60H+ in the presence of trifluoroacetic acid to yield the final products 10-methylacridinium ion (AcrH+) and 1,2-C60H2. The transient spectra of the radical ion pair formed in the photoinduced electron transfer have been detected successfully in laser flash photolysis of each NADH analog-C60 system. The mechanistic difference between the selective one- and two-electron redns. of C60 is discussed on the basis of the difference in the redox and acid-base properties of NADH and the dimer analogs.

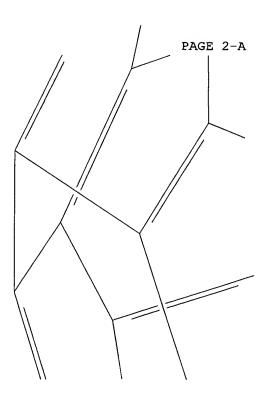
IT 160482-48-4P

RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(selective one-electron and two-electron reduction of C60 with NADH and NAD dimer analogs via photoinduced electron transfer)

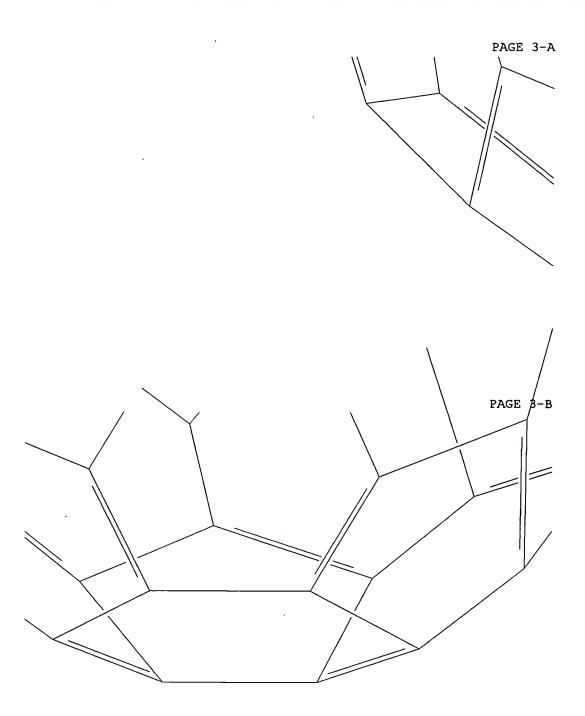
- RN 160482-48-4 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-(9CI) (CA INDEX NAME)
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
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RE.CNT 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

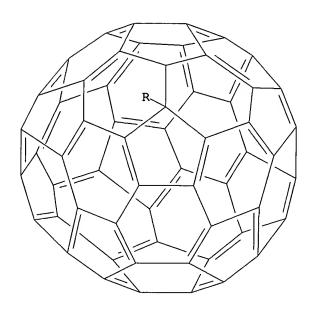
- L5 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:439511 CAPLUS
- DN 129:208728
- TI Photoluminescence of fullerene [60] in ultrathin ordered multilayers: the dissociation of molecular aggregation
- AU Ma, Shihong; Lu, Xingze; Xu, Jianhua; Cai, Zhigang; Zhou, Jianying; Wang, Wencheng; Zhang, Zhiming
- CS State Key Joint Laboratory for Materials Modification by Laser, Ion and Electron Beams, Department of Physics, Fudan University, Shanghai, 200433, Peop. Rep. China
- SO Chinese Science Bulletin (1998), 43(12), 1004-1008 CODEN: CSBUEF; ISSN: 1001-6538
- PB Science in China Press
- DT Journal
- LA English
- AB The aggregation behavior of a substituted fullerene compound, 1-benzyl-2-hydro[60] fullerene (C60-Be), in Z-type ultrathin ordered (e.g. LB) multilayers was studied by UV-visible absorption, steady state and time-resolved fluorescence spectroscopies. The LB multilayers of pure C60-Be showed J-aggregate formation, characterized by a large red shift of two absorption peaks (ΔΕ.apprx.2,098 cm-1 from 260-275 nm and ΔΕ.apprx.1,076 cm-1 from 328-340 nm, resp.). The main fluorescence emission bands were found at 710, 646, 603, 600 and 595 nm for pure C60-Be, mixed C60-Be (molar percentage 50%, 25% and 20%, resp.) multilayers and monomeric C60-Be, mixed C60-Be (molar percentage 50%, 25% and 20%, resp.) in LB films could be best-fitted by using a bi-exponential decay model.

IT 170646-75-0

RL: OCU (Occurrence, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); OCCU (Occurrence); PROC (Process) (photoluminescence of fullerene [60] in ultrathin ordered multilayers and dissociation of mol. aggregation)

- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

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CH2-Ph

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 11 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:282928 CAPLUS
- DN 129:27672
- TI Synthesis and Spectroscopic and Electrochemical Characterization of Diand Tetrasubstituted C60 Derivatives
- AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Hirasaka, Takeomi; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Journal of Physical Chemistry A (1998), 102(22), 3898-3906 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English
- The synthesis and electrochem. and spectroscopic characterization of fullerene derivs. of the type R2C60 where R = C6H5CH2, 2-BrC6H4CH2, 3-BrC6H4CH2, or 4-BrC6H4CH2 and R4C60 where R = C6H5CH2 are reported. The first step in the synthesis involves an electron transfer between C602-and RBr, and a similar initial electron-transfer step occurs between [(C6H5CH2)2C60]2- and C6H5CH2Br during the synthesis of (C6H5CH2)4C60. On the basis of NMR and UV-visible data, the investigated R2C60 derivs. are identified as 1,4-adducts of C60, whereas the isolated isomer of (C6H5CH2)4C60 is characterized as possessing C1 symmetry with the four benzyl groups being close to each other. The electrochem. of each synthesized compound was determined in benzonitrile containing 0.1 M

10/721,318 (RCE)

tetra-n-butylammonium perchlorate and each mono- and dianion of R2C60 and R4C60 were characterized by near-IR spectroscopy. The near-IR spectra of each species show two major "marker bands" which can be considered to be diagnostic of the fullerene derivative oxidation state.

IT 207684-64-8

CN

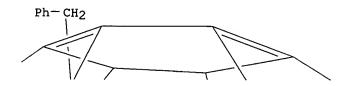
RL: PRP (Properties)

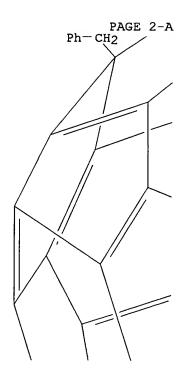
(calculated LUMO structure; synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

RN 207684-64-8 CAPLUS

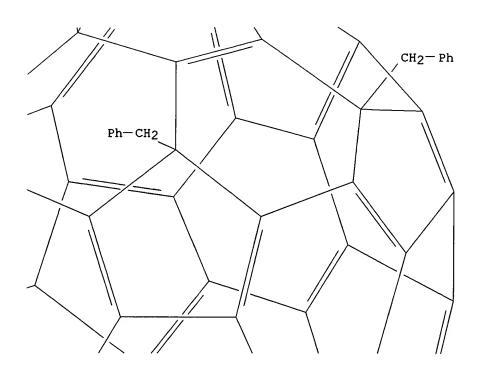
[5,6]Fullerene-C60-Ih, 1,6,11,18-tetrahydro-1,6,11,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

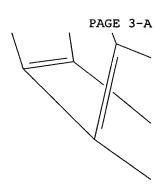
PAGE 1-A

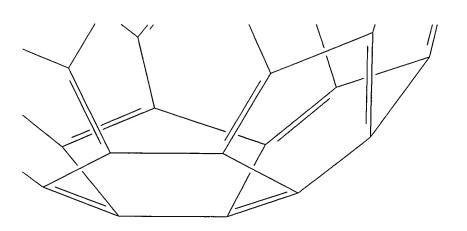












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IT 207684-63-7

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (synthesis and spectroscopic and electrochem. characterization of diand tetrabenzylated C60 derivs.)

RN 207684-63-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2,3,13-tetrahydro-3,13-bis(phenylmethyl)-, ion(2-) (9CI) (CA INDEX NAME)

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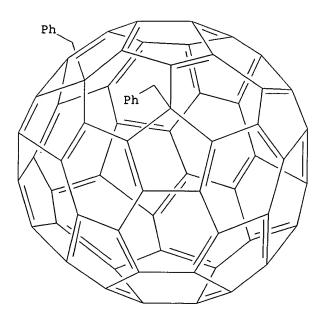
IT 182212-24-4 195625-44-6 195625-45-7 195625-46-8 207684-65-9 207684-66-0 207684-67-1

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

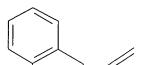
(synthesis and spectroscopic and electrochem. characterization of diand tetrabenzylated C60 derivs.)

RN 182212-24-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)

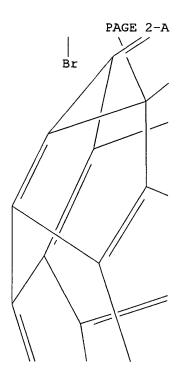


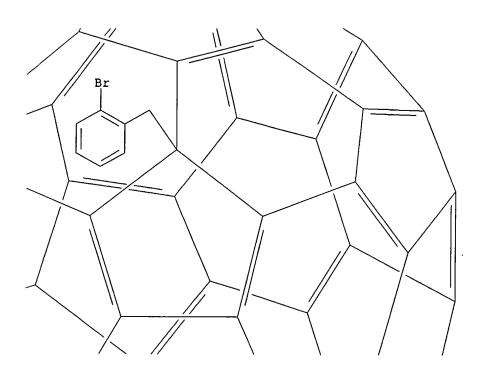
RN 195625-44-6 CAPLUS
CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)



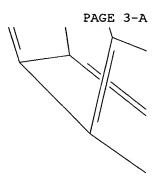
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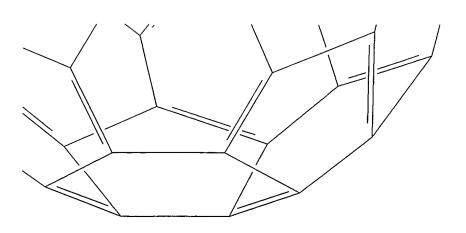






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RN 195625-45-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 195625-46-8 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)

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RN 207684-65-9 CAPLUS

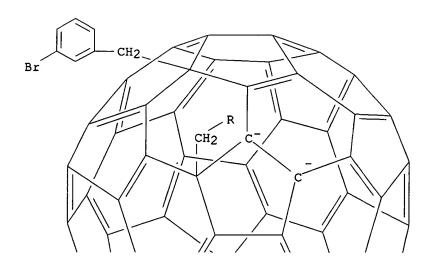
CN [5,6]Fullerene-C60-Ih, 3,13-bis[(2-bromophenyl)methyl]-1,2,3,13-tetrahydro-, ion(2-) (9CI) (CA INDEX NAME)

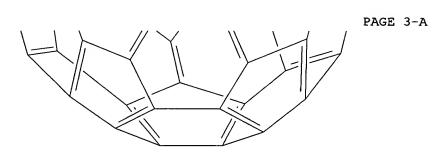
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RN 207684-66-0 CAPLUS

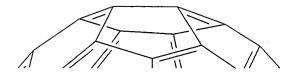
CN [5,6]Fullerene-C60-Ih, 3,13-bis[(3-bromophenyl)methyl]-1,2,3,13-tetrahydro-, ion(2-) (9CI) (CA INDEX NAME)



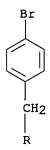




RN 207684-67-1 CAPLUS
CN [5,6]Fullerene-C60-Ih, 3,13-bis[(4-bromophenyl)methyl]-1,2,3,13-tetrahydro-, ion(2-) (9CI) (CA INDEX NAME)



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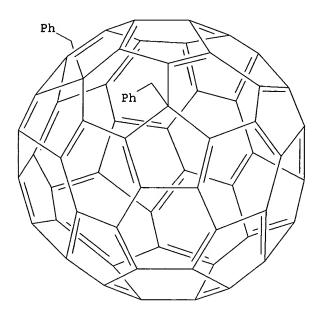
IT 176106-61-9P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(synthesis and spectroscopic and electrochem. characterization of diand tetrabenzylated C60 derivs.)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 195625-41-3P 195625-42-4P 195625-43-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and spectroscopic and electrochem. characterization of diand tetrabenzylated C60 derivs.)

RN 195625-41-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 195625-42-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro- (9CI)

(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 195625-43-5 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

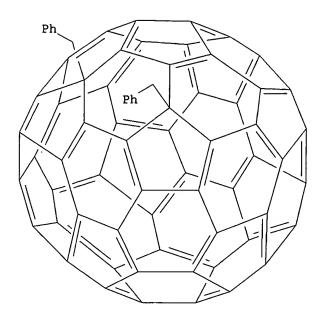
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 12 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1998:273225 CAPLUS
- DN 129:40968
- TI Synthesis and characterization of [(C6H5CH2)4C60]n- where n = 0, 1 or 2
- AU Gao, Xiang; Van Caemelbecke, Eric; Materazzi, Stefano; Kadish, Karl M.; Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, Takeomi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Proceedings Electrochemical Society (1997), 97-42(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, Vol. 5), 99-116
 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- The synthesis, electrochem. and spectroscopic characterization of (C6H5CH2)4C60 is reported. A mechanism for the synthesis starting from (C6H5CH2)2C60 is proposed and involves an initial electron transfer between [(C6H5CH2)2C60]2- and C6H5CH2Br followed by a radical coupling process. Mass spectra and 1H NMR data indicate that several isomers of (C6H5CH2)4C60 are generated during the reaction and two of these are characterized in this paper as possessing C1 symmetry with the four benzyl groups being close to each other. Near IR spectra for one of the isomers of [(C6H5CH2)4C60]- and [(C6H5CH2)4C60]2- are reported and compared with spectra for mono- and dianionic C60 and (C6H5CH2)2C60. Electrochem. data are also reported for one of the two isolated (C6H5CH2)4C60 isomers.
- IT 176106-61-9

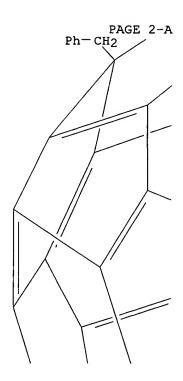
RL: RCT (Reactant); RACT (Reactant or reagent)
 (benzylation of dibenzylfullerene)

- RN 176106-61-9 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



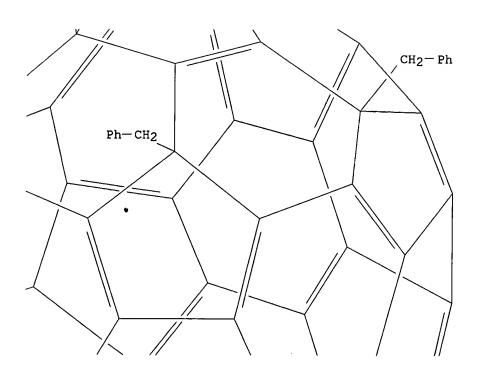
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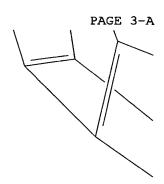


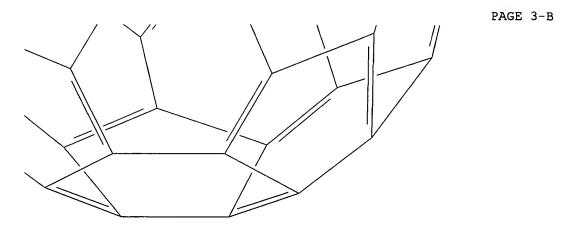


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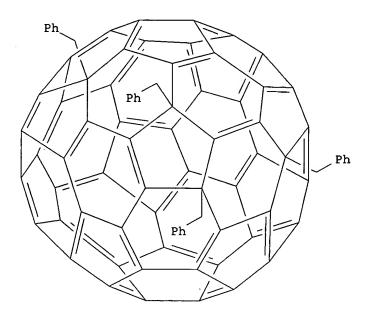
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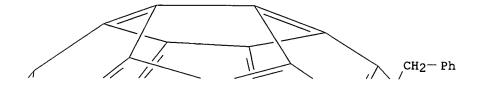


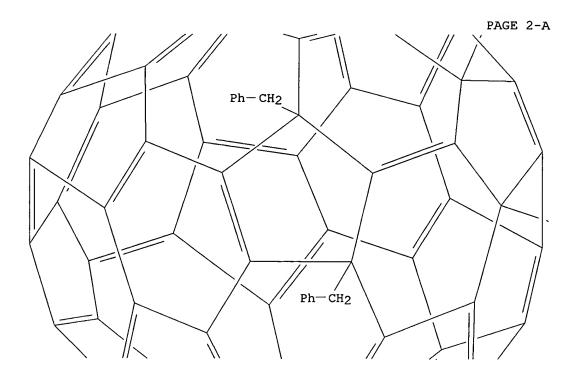


RN 208119-55-5 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,3,7,13-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)



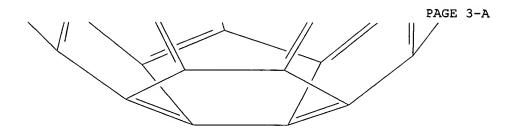
RN 208119-56-6 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,3,11,13-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)





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CH2-Ph

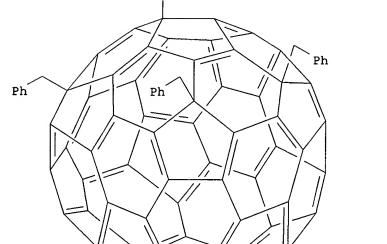


RN 208119-58-8 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,7,15,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

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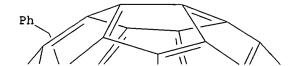
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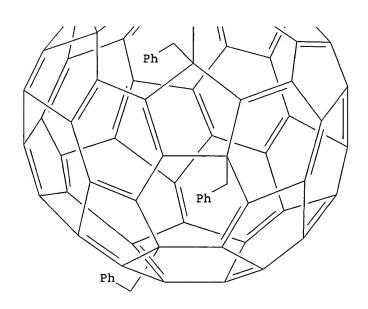


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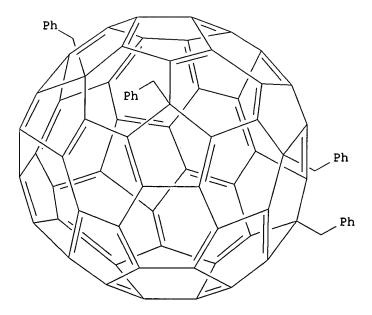
RN 208119-60-2 CAPLUS [5,6]Fullerene-C60-Ih, 1,3,7,17-tetrakis(phenylmethyl)- (9CI) (CA INDEX CN NAME)



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RN 208119-62-4 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,7,13,32-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)



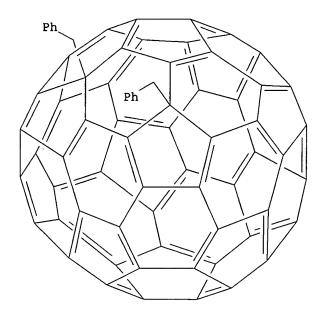
IT 182212-26-6

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(kinetics of reactions of dibenzylfullerene diamion and related compds. with alkyl halides)

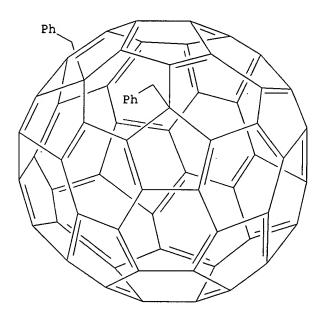
RN 182212-26-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-) (9CI) (CA INDEX NAME)



IT 182212-24-4

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)



RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 13 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1997:780509 CAPLUS
- DN 128:173507
- TI Photophysical investigation on molecular aggregation of 1-benzyl-2-hydro[60] fullerene in Langmuir-Blodgett multilayers
- AU Ma, Shihong; Lu, Xingze; Xu, Jianhua; Zhou, Guangpeng; Cai, Zhigang; Zhou, Jianying; Wang, Wencheng; Li, Yufen
- CS Department of Physics, Ion and Electron Beams, State Key Joint Laboratory for Materials Modification by Laser, Fudan University, Shanghai 200433, Peop. Rep. China
- SO Chemical Physics Letters (1997), 280(3,4), 308-314 CODEN: CHPLBC; ISSN: 0009-2614
- PB Elsevier Science B.V.
- DT Journal
- LA English
- AB The aggregation behavior of a substituted fullerene compound, 1-benzyl-2-hydro[60] fullerene (C60-Bh), in Z-type Langmuir-Blodgett (LB) multilayers was studied by UV-visible absorption, steady-state and time-resolved fluorescence spectroscopies. The LB multilayers of pure C60-Bh showed J-aggregate formation, characterized by a large red shift of 2 absorption peaks (ΔΕ.apprx.2098 cm-1 from 260-275 nm and ΔΕ.apprx.1076 cm-1 from 328-340 nm). The main fluorescence emission bands were found at 710, 646, 603 and 595 nm for pure C60-Bh, mixed C60-Bh/arachidic acid (AA) (1:1), mixed C60-Bh/nitrogencrown (NC) (1:3) multilayers and monomeric C60-Bh in solution, resp. The aggregates were dissociated by mixing with AA or NC. The fluorescence decay profiles of C60-Bh, C60-Bh/AA and C60-Bh/NC in LB films could be fitted by a

10/721,318 (RCE)

bi-exponential decay model.

IT 170646-75-0 202921-96-8 202921-98-0

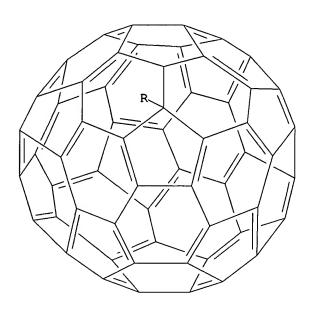
RL: PRP (Properties)

(mol. aggregation in Langmuir-Blodgett multilayers of)

RN 170646-75-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

RN 202921-96-8 CAPLUS

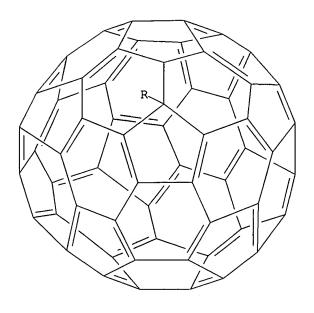
CN Eicosanoic acid, compd. with 1,9-dihydro-1-(phenylmethyl)[5,6]fullerene-C60-Ih (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170646-75-0

CMF C67 H8

PAGE 1-A



PAGE 2-A

CH2-Ph

CM 2

CRN 506-30-9 CMF C20 H40 O2

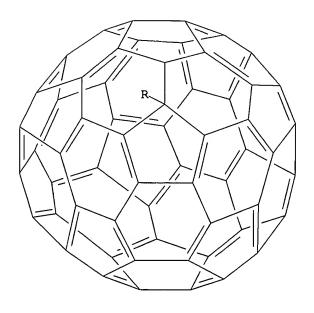
 ${
m HO_2C^-}$ (CH₂)₁₈-Me

RN 202921-98-0 CAPLUS
CN 1,4,7,10,13,16-Hexaazacyclooctadeca-1,3,10,12-tetraene,
7,16-bis(1-oxooctadecyl)-, compd. with 1,9-dihydro-1(phenylmethyl)[5,6]fullerene-C60-Ih (3:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170646-75-0 CMF C67 H8

PAGE 1-A



PAGE 2-A

CM 2

CRN 142706-29-4 CMF C48 H90 N6 O2

L5 ANSWER 14 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:556509 CAPLUS

DN 127:176128

 ${\tt TI}$ Quantum chemical studies on the structure and spectra of the addition product HC60CH2C6H5

10/721,318 (RCE)

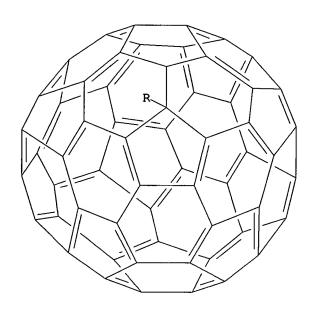
- AU Chen, Zhong-Fang; Teng, Qi-Wen; Wu, Shi; Pan, Yin-Ming; Zhao, Xue-Zhuang; Tang, Au-Chin; Feng, Ji-Kang
- CS Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China
- SO Gaodeng Xuexiao Huaxue Xuebao (1997), 18(8), 1346-1349 CODEN: KTHPDM; ISSN: 0251-0790
- PB Gaodeng Jiaoyu Chubanshe
- DT Journal
- LA Chinese
- AB The INDO series methods have been used to study the structures for the two kinds of isomers, which are 1,2-addition and 1,4-addition of HC60CH2C6H5. It
- indicated that 1,2-HC60CG2C6H5 has Cs symmetry, while 1,4-HC60CH2C6H5 has no symmetry. Furthermore, the total energy of 1,2-isomer is higher than that of 1,4-isomer. The electronic spectra for both isomers have been calculated based on the optimized geometries and the reason for the red-shift of the spectra has been discussed.
- IT 170646-75-0 194145-24-9

RL: PRP (Properties)

(MO calcn. of structure and UV of addition product HC60CH2C6H5)

- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



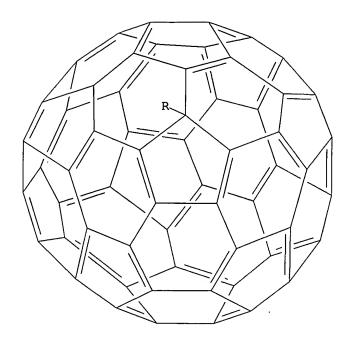


PAGE 2-A

CH2-Ph

- RN 194145-24-9 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

L5 ANSWER 15 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:551237 CAPLUS

DN 127:247723

TI Photoreactions with fullerenes

AU Mattay, Jochen; Siedschlag, Christina; Torres-Garcia, Gregorio; Ulmer, Lars; Wolff, Christian; Fujitsuka, Mamoru; Watanabe, Akira; Ito, Osamu; Luftmann, Heinrich

CS Institut fur Organische Chemie, Universitat Kiel, Kiel, D-24098, Germany

Proceedings - Electrochemical Society (1997), 97-14 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 326-337 CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal; General Review

LA English

AB The synthesis of azafulleroids and aziridinofullerenes is reported. Generally azafulleroids are formed upon thermolysis from azides. The corresponding aziridinofullerenes are obtained from the azafulleroids by irradiation, probably via a di-π-methane rearrangement. Surprisingly [70] fullerene gives only two isomeric azafulleroids with Cs-symmetry. The photoreactions of 4-methyl-1,2,4-triazoline-3,5-dione (NMTAD) with various [60] fullerene derivs. have been studied. In general, [60] fullerenes with a closed structure cycloadd in a [2+2] fashion to NMTAD whereas 1,6-methano-[60] fulleroid undergoes a [2+2+2] cycloaddn. also in the

10/721,318 (RCE)

absence of light. Finally new preparative results and some preliminary time-resolved laser flash photolysis studies on the generation and the reactions of [60] fullerene radical cations are reported; 27 refs.

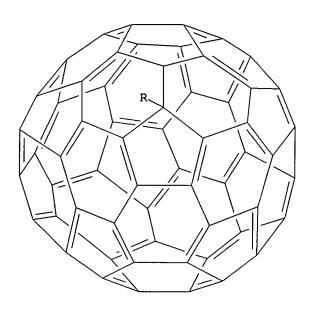
IT 170646-75-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (photochem. functionalization of C60)

RN 170646-75-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)





PAGE 2-A

CH2-Ph

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 16 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1997:551224 CAPLUS
- DN 127:247828
- TI Electrogeneration, electrochemistry and spectroelectrochemistry of C60 adducts
- AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Hirasaka, Takeomi; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Proceedings Electrochemical Society (1997), 97-14(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 221-235
 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal

LA English

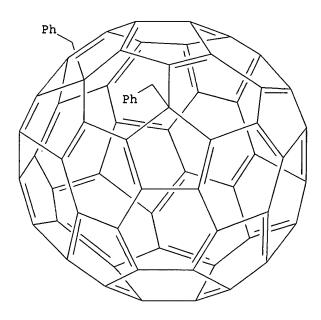
AB The synthesis, electrochem. and spectral characterization of fullerene derivs. of the type C60(R)2, where R = C6H5CH2, 2-BrC6H4CH2, 3-BrC6H4CH2 or 4-BrC6H4CH2 is reported. Near-IR absorptions for both monoanions and dianions of the investigated compds. are blue- and red-shifted with respect to the near-IR absorptions of C60- and C602-, resp. C60(C6H5CH2)4 was also electro-synthesized and characterized by mass spectrometry, 1H NMR, 13C NMR, UV-visible spectroscopy and electrochem. The isolated compound has a C1 symmetry and a possible structure is discussed on the basis of NMR and UV-visible data.

IT 182212-24-4P 182212-26-6P 195625-44-6P 195625-45-7P 195625-46-8P 195738-81-9P 195738-82-0P 195738-83-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (near IR spectra of C60 adduct anions)

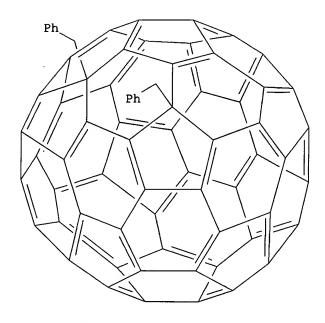
RN 182212-24-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)

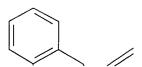


RN 182212-26-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-) (9CI) (CA INDEX NAME)

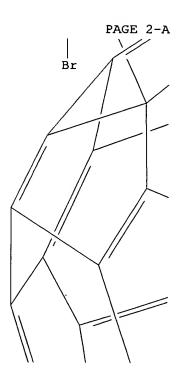


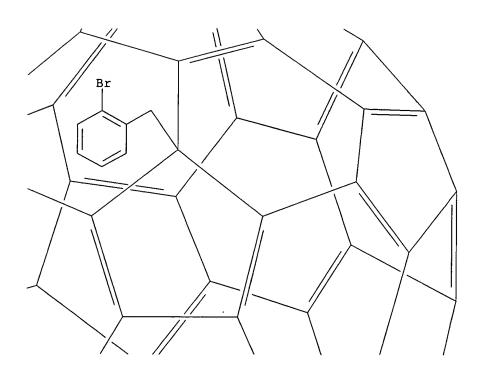
RN 195625-44-6 CAPLUS
CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)



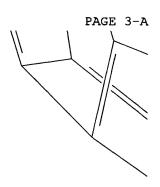
PAGE 1-B

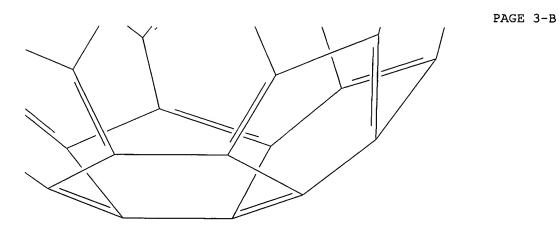






PAGE 2-B





RN 195625-45-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

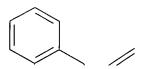
RN 195625-46-8 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-, radical ion(1-) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

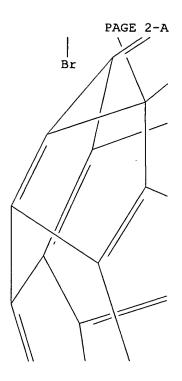
RN 195738-81-9 CAPLUS

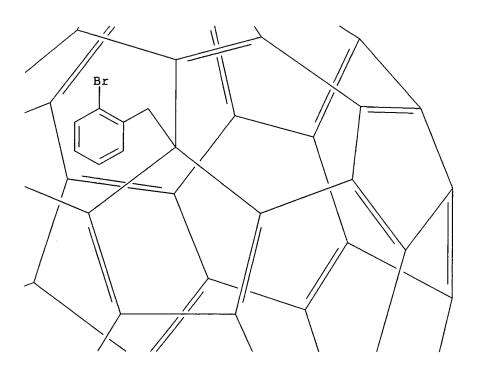
CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-, radical ion(2-) (9CI) (CA INDEX NAME)



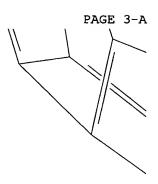
PAGE 1-B

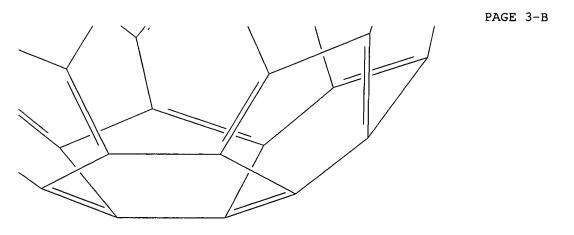






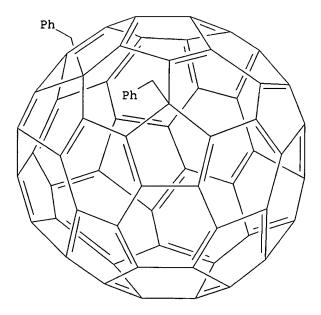
PAGE 2-B





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RN
     195738-82-0 CAPLUS
CN
     [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-,
     radical ion(2-) (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN
     195738-83-1 CAPLUS
CN
     [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-,
     radical ion(2-) (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     176106-61-9P 195625-41-3P 195625-42-4P
IT
     195625-43-5P
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
     (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC
     (Process); RACT (Reactant or reagent)
        (synthesis, electrochem. and spectral characterization of fullerene
        derivs)
     176106-61-9 CAPLUS
RN
     [5,6] Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX
CN
```

NAME)



RN 195625-41-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 195625-42-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 195625-43-5 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 17 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1997:551220 CAPLUS
- DN 127:234001
- TI Generation of C60 adducts with two different alkyl groups in the reactions between C2-60 and alkyl halides
- AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, Takeomi; Gao, Xiang; Van Caemelbecke, Eric; Kadish, Karl M.
- CS Department of Applied Chemistry, Faculty of Engineering, Osaka University, Suita, 565, Japan
- SO Proceedings Electrochemical Society (1997), 97-14(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 173-185
 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- AB Symposium proceedings. The C602- generated in the reduction of C60 with

10/721,318 (RCE)

naphthalene radical anion in benzonitrile reacts with various alkyl halides (RX) to yield the corresponding mono-alkyl adduct anions RC60-. An extensive comparison of the rate consts. for the alkylation of C2-60 with RX with those of electron transfer from tetramethylsemiquinone radical anion to the same series of RX demonstrates clearly that electron transfer from C2-60 to RX is the rate-determining step in the alkylation of C602-. A mono-alkyl adduct anion, t-BuC60-, produced in the reaction of C602- with t-BuI undergoes no further reaction with t-BuI, but the SN2 reaction proceeds with less sterically hindered RX to produce dialkyl-substituted C60 with different alkyl groups, i.e., (t-Bu)(C6H5CH2)C60. Protonation of t-BuC60- with trifluoroacetic acid occurs to produce (t-Bu) HC60. Extensive kinetic studies on the reactions of t-BuC60- with RX are compared with those for the authentic SN2 reactions of cobalt(I) tetraphenylporphyrin anion with RX and reveal that the reactions of t-BuC60- with RX proceed via a SN2 pathway rather than an electron transfer pathway. The difference in reactivities between the electron transfer and SN2 reactions enable us to prepare dialkyl-substituted C60 with two different alkyl groups.

IT 182070-59-3

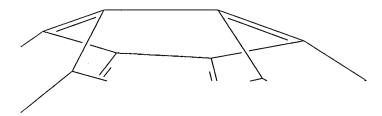
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(kinetics and mechanism of 2-step alkylation of fullerene dianion with alkyl halides)

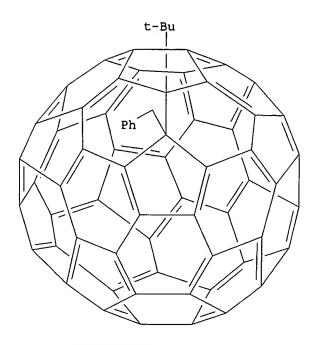
RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-B



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- IT 195392-52-0
 - RL: PRP (Properties)
 - (kinetics and mechanism of 2-step alkylation of fullerene dianion with alkyl halides)
- RN 195392-52-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,9-dihydro-9-(phenylmethyl)-(9CI) (CA INDEX NAME)



IT 160482-48-4P

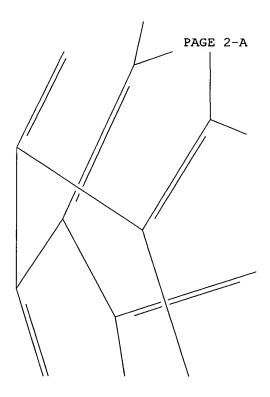
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (kinetics and mechanism of 2-step alkylation of fullerene dianion with alkyl halides)

RN 160482-48-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-(9CI) (CA INDEX NAME)

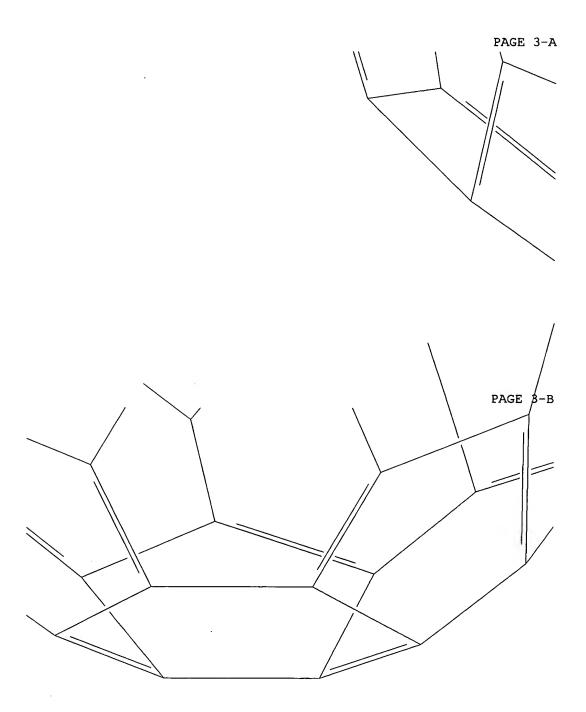
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 1-C



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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *



PAGE 3-C



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

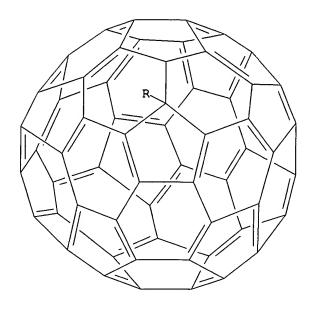
- L5 ANSWER 18 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1997:523807 CAPLUS
- DN 127:240547
- TI Fabrication and optical nonlinearities of Langmuir-Blodgett multilayers of 1-benzyl-9-hydrofullerene-60
- AU Ma, Shihong; Lu, Xingze; Han, Kui; Liu, Liying; Wang, Gongming; Wang, Wencheng; Li, Yufen; Chen, Jian; Cai, Ruifang; Huang, Zu'en
- CS Dep. Phys., Fudan Univ., Shanghai, 200433, Peop. Rep. China
- SO Guangxue Xuebao (1996), 16(11), 1600-1606 CODEN: GUXUDC; ISSN: 0253-2239
- PB Kexue
- DT Journal
- LA Chinese
- AB The structural features of the Langmuir-Blodgett (LB) films of substituted fullerene C60-Be was studied by π -A isotherm, small angle x-ray diffraction (SAXD), and optical measurements. Pure C60-Br mols. at the air-H2O interface in a bulk phase were found. 1,10-Bis(stearyl)-4,6,13,15-tetraene-18-nitrogencrown-6 (NC) was used as an inert material to construct mixed C60-Be/NC LB films which had a much better quality than the pure C60-Be LB films. The structural improvement in the mixed C60-B/NC LB films was realized by π -A isotherm, UV-visible absorption, and SAXD measurements as an insertion of C60-Be mols. between the two chains of NC. The 3rd-order nonlinear susceptibility XXXXX(3) is $(-3\omega;\omega,\omega,\omega) = 2.1 + 10-11$ esu by the method of three-harmonic generation in mixed C60-Be/NC LB films.
- IT 170646-75-0

RL: PRP (Properties)

(fabrication and optical nonlinearities of Langmuir-Blodgett multilayers of 1-benzyl-9-hydrofullerene-60 with crown derivative)

- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

L5 ANSWER 19 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:479924 CAPLUS

DN 127:240782

TI Enhanced coalescence reactions of fullerenes by laser desorption of C60 derivatives

AU Ong, P. P.; Zhu, Lei; Zhao, Li; Zhang, Jun; Wang, Shenyi; Li, Yufen; Cai, Ruifang; Huang, Zuen

CS Dep. of Phys., Natl. Univ. of Singapore, Singapore, 0511, Singapore

SO International Journal of Mass Spectrometry and Ion Processes (1997), 163(1,2), 19-28
CODEN: IJMPDN; ISSN: 0168-1176

PB Elsevier

DT Journal

LA English

AB We observed enhanced coalescence reactions of fullerenes by laser desorption of chemical adducts of (C6HCH2)nC60, (C9H7)mHnC60, (CCl2)xC60 and the newly available poly-N-vinylcarbazole (PVK)-C60/70. The mass spectra of the laser-produced species reveal a characteristic bi-modal profile, with one maximum abundance distribution of parent fullerene ions located at C60 and the other at nearly twice C60. The mass spectra of both pristine C60 and the non-reactive PS/C60 mixture show monotonically descending intensity of daughter fullerenes with successive C2 captures, whereas slightly enhanced coalescence products are observed for the reactive PVK/C60/70 mixture which is known as a charge transfer complex. The mechanism of efficient coalescence is believed to be cluster collisional nucleation of pairs of reactive fullerene fragments (nascent C60, C58, etc.) induced by photofragmentation of the reactive Rn-C60 adduct or

 ${\tt Rn\cdot\cdot\cdot C60}$ charge transfer system, which is indicated by the laser power dependence features and the correlation between enhanced fullerene fragments and coalescence products.

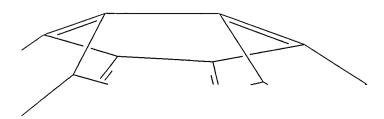
IT 140656-83-3P

RL: ANT (Analyte); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process)

(enhanced coalescence reactions of fullerenes by laser desorption of C60 derivs.)

RN 140656-83-3 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
 RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L5 ANSWER 20 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1997:110816 CAPLUS
- DN 126:144421
- TI Addition reaction of allylic stannanes to the triplet excited state of C60 via photoinduced electron-transfer process leading to asymmetric hybridization chemistry for fullerene terpenoid
- AU Mikami, Koichi; Matsumoto, Shoji; Tonoi, Takayuki; Suenobu, Tomoyoshi; Ishida, Akito; Fukuzumi, Shunichi
- CS Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo, 152, Japan
- SO Synlett (1997), (1), 85-87 CODEN: SYNLES; ISSN: 0936-5214
- PB Thieme
- DT Journal
- LA English

- OS CASREACT 126:144421
- AB Addition of allylic stannanes to C60 takes place under UV-irradiation in C6H6 or

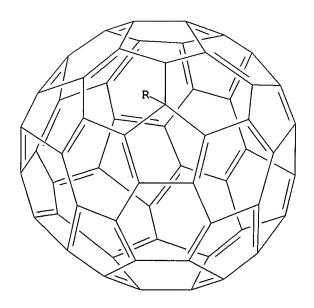
PhCN to yield the allylic fullerenes. An enantiopure fullerene terpenoid was obtained when a pinene-derived allylic stannane was used.

- IT 186696-07-1P
 - RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of allylfullerenes by photoaddn. of allylic stannanes to C60)

- RN 186696-07-1 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1-[(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl]-1,9-dihydro-, (-)- (9CI) (CA INDEX NAME)
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- L5 ANSWER 21 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:677390 CAPLUS
- DN 126:24514
- TI Efficient optical nonlinear Langmuir-Blodgett films: Roles of matrix molecules
- AU Ma, Shihong; Lu, Xingze; Liu, Liying; Han, Kui; Wang, Wencheng; Zhang, Zhiming
- CS Department Physics, Fudan University, Shanghai, 200433, Peop. Rep. China
- Proceedings of SPIE-The International Society for Optical Engineering (1996), 2897 (Electro-Optic and Second Harmonic Generation Materials, Devices, and Applications), 59-67 CODEN: PSISDG; ISSN: 0277-786X
- PB SPIE-The International Society for Optical Engineering
- DT Journal
- LA English
- AB A novel bifat-chain amphiphilic mol. nitrogen-crown (NC) was adopted as an inert material for fabrication of optical nonlinear Langmuir-Blodgett (LB) multilayers. Structural improvement in the Z-type mixed fullerene derivative (C60-Be)/NC LB multilayers samples was realized by insertion of the C60-Be mols. between two hydrophobic chains of the NC mols. The relatively large 3rd-order susceptibility χ(3) xxxx(-3ω;ω,ω,ω) = 2.9 + 10-19 M2V2 (or 2.1 + 10-11 esu) was deduced by measuring 3rd harmonic generation (THG) from the C60-Be samples. The 2nd harmonic generation (SHG) intensity increased quadratically with the bilayer number (up to 116 bilayers) in Y-type hemicyanine (HEM)/NC interleaving LB multilayers due to improvement of the structural properties by insertion of the long hydrophobic tail of HEM mols. between two chains of NC mols. The 2nd-order susceptibility χ(2) zxx(-2ω;ω,ω) = 18
 pM V-1 (or 4.35 + 10-8 esu) was obtained by measuring SHG from the
 - pM V-1 (or 4.35 + 10-8 esu) was obtained by measuring SHG from the HEM samples. The NC mol. has attractive features as a matrix material in fabrications of LB multilayers made from optically nonlinear materials with hydrophobic long tails or ball-like mols.
- IT 170646-75-0
 - RL: OCU (Occurrence, unclassified); PRP (Properties); OCCU (Occurrence) (efficient optical nonlinear Langmuir-Blodgett films and their properties and role of matrix mols.)
- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

L5 ANSWER 22 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:570714 CAPLUS

DN 125:300590

TI Chemical generation of C60 anions and the alkylation with alkyl halides via electron transfer

AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Kadish, K. M.; Subramanian, R.; Jones, M. T.

CS Dep. Appl. Chem., Osaka Univ., Osaka, 565, Japan

Proceedings - Electrochemical Society (1996), 96-10 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, Vol. 3), 243-252
CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

The naphthalene radical anion was used as an electron transfer reductant to reduce C60 to generate C60•-, C602-, and C60•3- in benzonitrile. The C602- thus generated reacts with various alkyl halides (RX) to yield the radical anions of the corresponding dialkyl derivs.

R2C60•-. The R2C60 was obtained after the workup. The 2nd-order rate consts. of the alkylation of C602- with various alkyl halides are determined by monitoring the decrease in absorbance due to C602-. The reactivity of RX is rather insensitive to the steric hindrance of the alkyl groups of RX, being opposite from what is expected for the normal reactivity in the SN2 reaction. Such insensitiveness to the steric hindrance is shown to agree well with the reactivity of RX in the electron transfer reduction by a 1-electron reductant. An extensive comparison between the rate consts. of

the alkylation of C602- with various RX and those of electron transfer from tetramethylsemiquinone radical anion to the same series of RX demonstrates clearly that electron transfer from C602- to RX is the rate-determining step in the alkylation of C602-. A novel reaction mechanism

οf

sequential electron transfer and SN2 is presented based on the kinetic studies on the alkylation of C602-, being specific to fullerene anions in which electrons are highly delocalized.

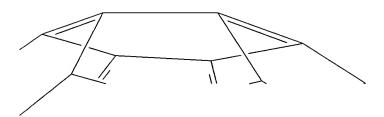
IT 182070-59-3

.RL: PRP (Properties)

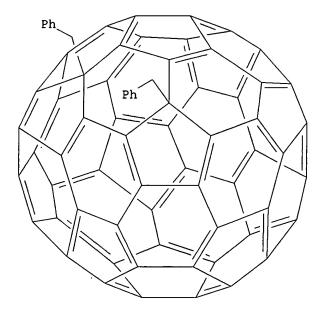
(PM3 calcn. of charge distribution in)

RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)



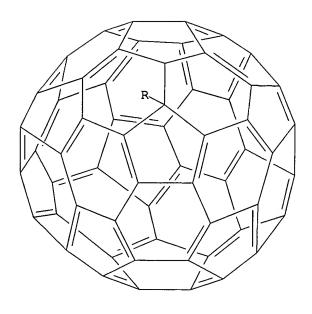
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- 176106-61-9P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- 176106-61-9 CAPLUS RN
- CN[5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



- L5 ANSWER 23 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:569590 CAPLUS
- DN 125:288019
- TI Structural and Optical Nonlinear Characterizations of Langmuir-Blodgett Films of 1-Benzyl-9-hydrofullerene-60
- AU Ma, Shihong; Lu, Xingze; Chen, Jian; Han, Kui; Liu, Liying; Huang, Zuen; Cai, Ruifang; Wang, Gongming; Wang, Wencheng; Li, Yufen
- CS Department of Physics, Fudan University, Shanghai, 200433, Peop. Rep. China
- SO Journal of Physical Chemistry (1996), 100(41), 16629-16632 CODEN: JPCHAX; ISSN: 0022-3654
- PB American Chemical Society
- DT Journal
- LA English
- The structural and optical nonlinear features of the condensed layers at the air-H2O interface and Langmuir-Blodgett (LB) films of the substituted fullerene 1-benzyl-9-hydrofullerene-60 (C60-Be) were studied by π -A isotherm, small angle x-ray diffraction (SAXD), and optical measurements. Pure C60-Be mols. existed at the air-H2O interface in a bulk phase. A new type of 2-chain amphiphilic mol., 1,10-bistearyl-4,6,13,15-tetraene-18-N-crown-6 (NC), was used as an inert material to construct mixed C60-Be/NC LB films of much better quality than the pure C60-Be LB films. π -A, UV-visible spectra, and SAXD measurements show that the structural improvement in the mixed C60-Be/NC LB films was realized by insertion of the C60-Be mols. between the 2 hydrophobic chains of the NC mols. The relatively large 3rd-order nonlinear susceptibility $\chi(3) \times \times \times (-3\omega; \omega, \omega, \omega) = 2.1 + 10-11$ esu was deduced by measuring 3rd-harmonic generation in the mixed C60-Be/NC LB films.
- IT 170646-75-0, 1-Benzyl-9-hydrofullerene-60
 - RL: PRP (Properties)
 - (structural and optical nonlinear properties of Langmuir-Blodgett films of)
- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX

NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

- L5 ANSWER 24 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:554872 CAPLUS
- DN 125:275067
- TI Chemical Generation of C602- and Electron Transfer Mechanism for the Reactions with Alkyl Bromides
- AU Subramanian, Ramakrishnan; Kadish, Karl M.; Vijayashree, Madakasira N.; Gao, Xiang; Jones, M. Thomas; Miller, Mitchell D.; Krause, Kurt L.; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641,
- SO Journal of Physical Chemistry (1996), 100(40), 16327-16335 CODEN: JPCHAX; ISSN: 0022-3654
- PB American Chemical Society
- DT Journal
- LA English
- AB A simple solution-phase method that uses chemical generated p-benzoquinone dianions (Q2-) as the reductant in the selective generation of either C60- or C602- is described. The electron transfer reduction of C60 by Q2- occurs via stepwise electron transfer from the Q2- to C60 in acetonitrile or benzonitrile. The C602- thus generated is used as the starting material in the synthesis of RxC60 (where x = 2 for R = C6H5CH2 and x = 1 for R = o-xylyl) by the reaction of C602- with benzyl bromide or α, α' -dibromo-o-xylene. Theor. calcns. predict that the 1,4-isomer of (C6H5CH2)2C60 should be selectively formed, and this is confirmed by single-crystal x-ray diffraction studies. UV-visible and

near-IR spectroscopy were used to monitor the progress of electron transfer from the Q2- to C60 as well as the subsequent reactions between C602- and the alkyl bromides. The comparison of the observed rate consts. of the reactions of C602- with those of electron transfer from tetramethylsemiquinone radical anion to the same alkyl bromide indicates that the formation of RxC60 proceeds via the rate-determining electron transfer from C602- to the alkyl bromide.

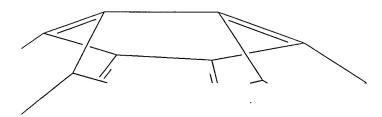
IT 182070-59-3 182070-67-3

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)



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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * RN 182070-67-3 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1-[[2-(bromomethyl)phenyl]methyl]-1,2-dihydro-, ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A



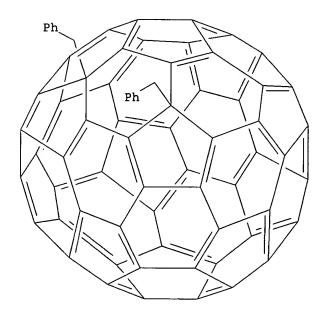
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * IT 182212-24-4 182212-26-6

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

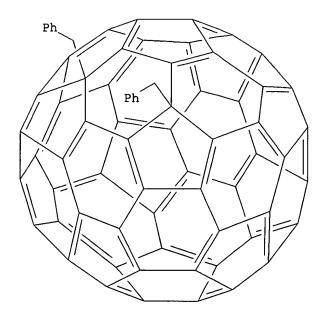
RN 182212-24-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)



RN 182212-26-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-) (9CI) (CA INDEX NAME)



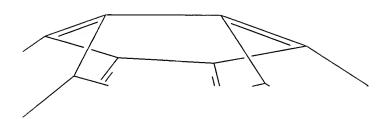
IT 172885-95-9 172990-44-2

RL: PRP (Properties)

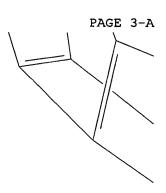
(chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

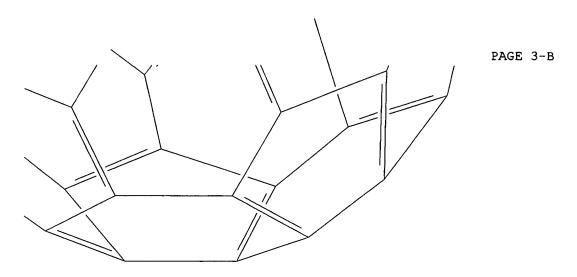
RN 172885-95-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

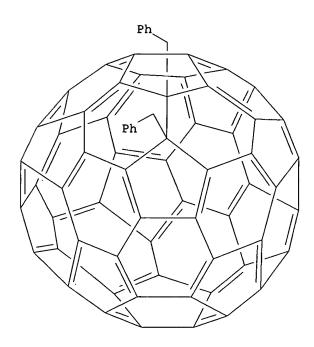


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RN 172990-44-2 CAPLUS CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1,9-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



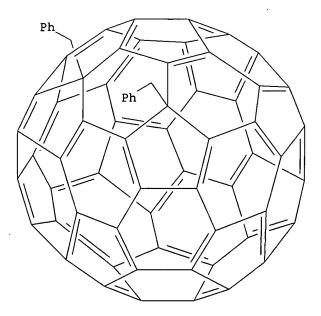
IT 176106-61-9P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(crystal and mol. structure; chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

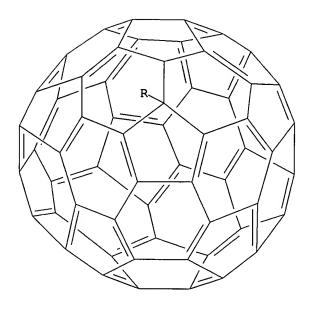
RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



- L5 ANSWER 25 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:356136 CAPLUS
- DN 125:114273
- TI Unusual reactions of C60 with aldehydes in the presence of aqueous ammonia
- AU Komori, Akifumi; Kubota, Masayuki; Ishida, Takayuki; Niwa, Haruki; Nogami, Takashi
- CS Dep. Appl. Phys. Chem., Univ. Electro-Commun., Chofu, 182, Japan
- SO Tetrahedron Letters (1996), 37(23), 4031-4034 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier
- DT Journal
- LA English
- OS CASREACT 125:114273
- AB Fullerene C60 reacts with alkylaldehydes in the presence of aqueous ammonia to give 2,5-dialkyl-substituted pyrrolidine derivs. The reaction of phenylacetaldehyde under similar conditions afforded C60(H)(CH2Ph) via possible decarbonylation. On the basis of the product anal., reaction mechanisms are proposed in which C60 plays the role of a dipolarophile or radical scavenger.
- IT 170646-75-0P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (unusual reactions of C60 with aldehydes in the presence of aqueous ammonia)
- RN 170646-75-0 CAPLUS
- CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

CH2-Ph

- L5 ANSWER 26 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:212770 CAPLUS
- DN 124:342817
- TI Fullerene-acetylene hybrids: towards a novel class of molecular carbon allotropes
- AU Timmerman, Peter; Anderson, Harry L.; Faust, Ruediger; Nierengarten, Jean-Francois; Habicher, Tilo; Seiler, Paul; Diederich, Francois
- CS Lab. Org. Chem., ETH-Zentrum, Zurich, CH-8092, Switz.
- SO Tetrahedron (1996), 52(14), 4925-47 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier
- DT Journal
- LA English
- OS CASREACT 124:342817
- The synthesis and complete characterization of 17 new fullerene-acetylene covalent derivs. is described. Reaction of 3-bromo-1,5-bis(trimethylsilyl)penta-1,4-diyne with C60 gave bis-protected diethynylmethanofullerene (4) in 56% yield. Unsym. bis-protected diethynylmethanofullerene (6) was synthesized in 53% yield from tosylhydrazone [(i-Pr)3SiC.tplbond.CC(:NNHTos)C.tplbond.CSiMe3] and C60. Proto-desilylation of 4 and 6 gave the corresponding free alkynes (3 and 8) in 83% and 69% yield, resp. Partial deprotection of 4 afforded the mono-protected fullerene in 35% yield. Oxidative hetero-coupling reactions of 3 and 8 under Hay conditions with various monosubstituted acetylenes gave butadiynylmethanofullerenes (10-13) in yields varying from 25-49%. Homo-coupling of 8 produced dumbbell-shaped fullerene 14, the 1st dimeric fullerene that could be fully characterized. The x-ray crystal

structure anal. of 14 revealed little or no electronic interaction between the two fullerene spheres. Addition of lithium trimethylsilylacetylide to C60 gave access to 1-substituted-2-(trimethylsilylethynyl) fullerenes. The acidity of hydro(trimethylsilylethynyl) fullerene (16), synthesized in 58% yield, was studied as a function of base and solvent. Reaction of lithiated (trimethylsilylethynyl) fullerene (17) with various electrophiles is discussed. Alc. (trimethylsilylethynyl) fullerenemethanol (25) was prepared in 57% yield by reaction of 17 with formaldehyde. Under strongly basic conditions, 25 eliminates formaldehyde to give 16 in quant. yield. Oxidation of 25 afforded (trimethylsilylethynyl) fullerenecarboxaldehyde in 53% yield, a rather unstable compound that is easily converted to hydrofullerene 16. Conversion of 25 to the corresponding tosylate could be performed in 40% yield.

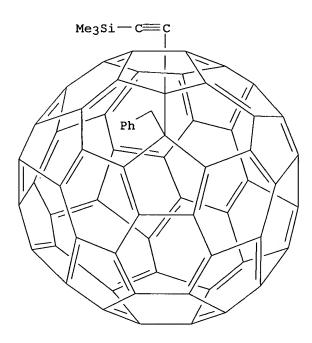
IT 175874-71-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fullerene-acetylene derivs.)

RN 175874-71-2 CAPLUS

CN Silane, trimethyl[[9-(phenylmethyl)[5,6]fulleren-C60-Ih-1(9H)-yl]ethynyl]-(9CI) (CA INDEX NAME)



IT 175874-75-6P

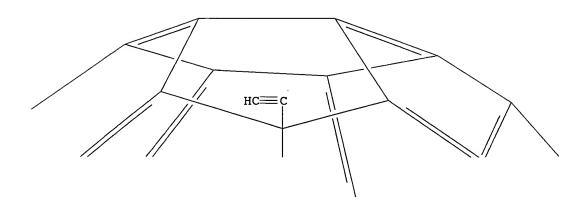
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of fullerene-acetylene derivs.)

RN 175874-75-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-ethynyl-1,9-dihydro-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



PAGE 1-B

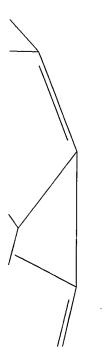


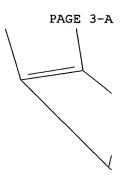
Page 95

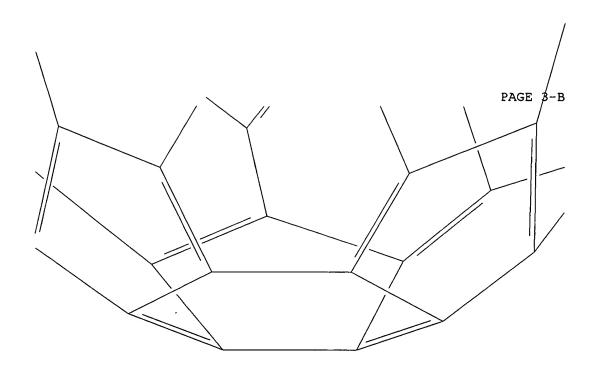
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PAGE 2-C







PAGE 3-C

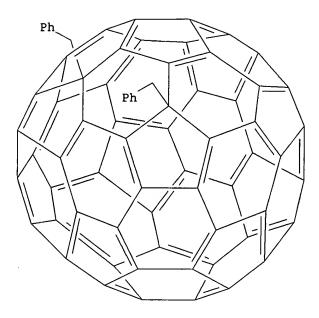


- L5 ANSWER 27 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:182541 CAPLUS
- DN 124:316718
- TI Introduction of two benzyl groups to C60 by using the Collman reagent
- AU Miki, Sadao; Kitao, Masunori; Fukunishi, Koushi
- CS Dep. Chemistry, Kyoto Inst. Technol., Kyoto, 606, Japan
- SO Tetrahedron Letters (1996), 37(12), 2049-52 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier
- DT Journal
- LA English
- OS CASREACT 124:316718
- AB Addition of C60 to a suspension of the Collman reagent in THF gave a strongly colored but almost transparent solution Treatment of the resulting solution with benzyl bromide gave a C60 derivative possessing two benzyl groups. The 1H-NMR as well as the 13C-NMR of the product indicated that the reaction site was 1,4-position.
- IT 176106-61-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (fullerene benzylation using Collman's reagent)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



- L5 ANSWER 28 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:127530 CAPLUS
- DN 124:288947
- Fullerene-acetylene molecular scaffolding: chemistry of 2-functionalized 1-ethynylated C60, oxidative homocoupling, hexakis-adduct formation, and attempted synthesis of C1242-
- AU Timmerman, Peter; Witschel, Lars E.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice
- CS Lab. Org. Chem., ETH-Zentrum, Zurich, CH-8092, Switz.
- SO Helvetica Chimica Acta (1996), 79(1), 6-20 CODEN: HCACAV; ISSN: 0018-019X
- PB Verlag Helvetica Chimica Acta
- DT Journal
- LA English
- AB On the way to the fullerene-acetylene hybrid carbon allotropes, the oxidative homocoupling of 2-functionalized 1-ethynylated C60 derivs. was investigated. Under Glaser-Hay conditions, two soluble dumbbell-shaped bisfullerenes with two C60 moieties 2,2'-substituted by PhCH2 or CH2OR (R = tetrahydropyranyl; I) linked by a butadiynediyl bridge were formed in 52 and 82% yield, resp. Cyclic-voltammetric measurements revealed that there is no significant electronic communication between the two fullerene spheres via the butadiynediyl linker. Removal of the protective groups in I gave in 80% yield a highly insol. dumbbell with methanol groups in the 2,2'-positions of the butadiynediyl-bridged carbon spheres. Attempted conversion of this compound to the corresponding all-carbon dianion C1242-via base-induced elimination of formaldehyde was not successful presumably due to exo-dig cyclization of the formed alkoxides. The occurrence of this cyclization under furan formation was proven for the soluble model

compound 2-[4-(trimethylsilyl)buta-1,3-diyn-1-yl][60]fullerene-1-methanol. To compare the properties of ethynylated fullerene mono-adducts to those of corresponding higher adducts, two hexakis-adducts with an octahedral functionalization pattern resulting from all-equatorial addns. were prepared by the reversible-template method of Hirsch. Reaction of ethynylated mono-adducts with 2-bromomalonate/DBU in the presence of 1,9-dimethylanthracene as reversible template led to hexakis-adducts in 28 and 22% yield. Preliminary expts. indicated a significant change in reactivity and NMR spectral properties of the fullerene addends with increasing degree of functionalization.

IT 175874-75-6

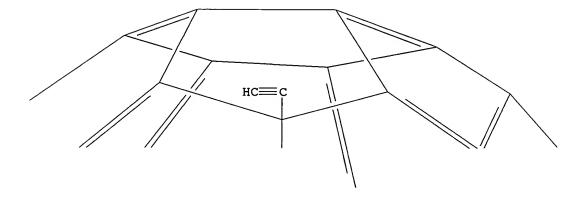
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of butadiynediyl-linked bisfullerenes and attempted conversion to dianion)

RN 175874-75-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-ethynyl-1,9-dihydro-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

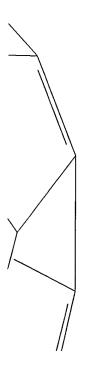
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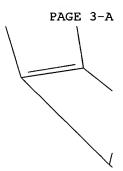


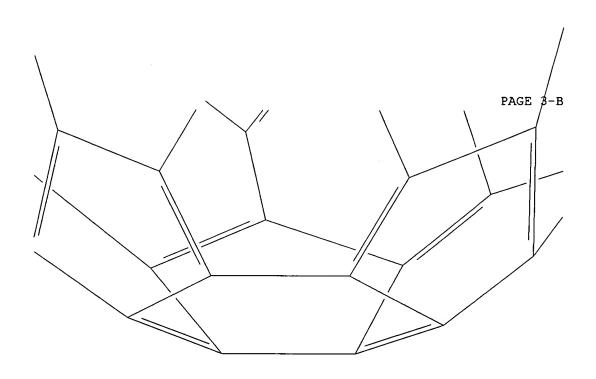
PAGE 1-C

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 2-C







PAGE 3-C

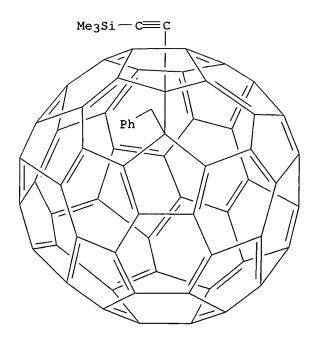


IT 175874-71-2P 175874-76-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (reduction potential; preparation of butadiynediyl-linked bisfullerenes and attempted conversion to dianion)

RN 175874-71-2 CAPLUS

CN Silane, trimethyl[[9-(phenylmethyl)[5,6]fulleren-C60-Ih-1(9H)-yl]ethynyl](9CI) (CA INDEX NAME)



RN 175874-76-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,1'-(1,3-butadiyne-1,4-diyl)bis[1,9-dihydro-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L5 ANSWER 29 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:991561 CAPLUS

DN 124:116838

TI Synthesis and characterization of (C6H5CH2)2C60 and related derivatives

AU Subramanian, R.; Vijayashree, M. N.; Mead, S. L.; Gao, X.; Jones, M. T.; Kadish, K. M.; Suenobu, T.; Fukuzumi, S.

CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA

SO Proceedings - Electrochemical Society (1995), 95-10(Proceedings of the Symposium on Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, 1995), 1150-63
CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

AB A simple, solution-phase chemical method which uses chemical generated hydroquinone

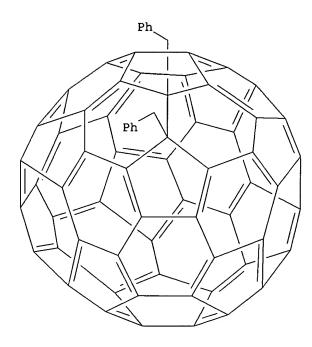
dianion as a reductant in the selective generation of either C60- or C602-is described. The C602- thus generated was used as the starting material in the synthesis of RxC60 where x=2 for R=C6H5CH2 and x=1 for R=co-xylyl. The products were characterized by 1H NMR spectroscopy which suggests that in the case of (C6H5CH2)2C60, only the 1,2-isomer (and not the thermodynamically favored 1,4-isomer) was obtained. UV-visible and near-IR spectroscopy were used to monitor the progress of electron transfer from the hydroquinone dianion to C60 as well as the subsequent reaction between C602- and the alkyl halide. Based on these results, a three step mechanism for the formation of RxC60 is proposed.

IT 172990-44-2P

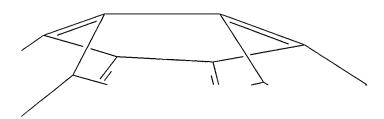
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and electrochem. reduction potentials of) RN 172990-44-2 CAPLUS

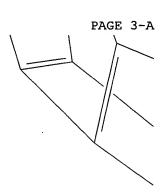
CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1,9-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

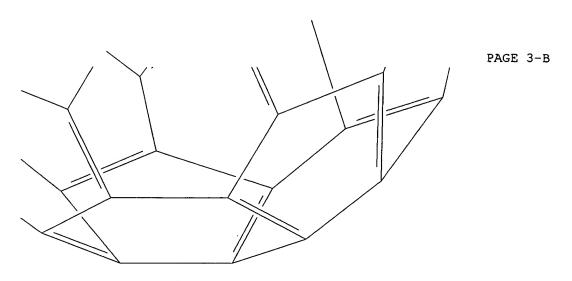


- L5 ANSWER 30 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:991467 CAPLUS
- DN 124:129665
- TI Electrochemistry, near-IR and ESR spectroscopy of $(R) \times C60$ where R = H, CH3, C6H5CH2 or o-xylyl
- AU Kadish, Karl M.; Boulas, Pierre L.; Vijayashree, M. N.; Subramanian, Ramakrishnan; Gao, Xiang; Mead, Steve; Tan, Zheng; Jones, M. Thomas
- CS Department Chemistry, University Houston, Houston, TX, 77204-5641, USA
- SO Proceedings Electrochemical Society (1995), 95-10(Proceedings of the Symposium on Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, 1995), 213-28 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- AB The authors report here the electrochem., near-IR and ESR spectroscopy of fullerene derivs. (R)xC60 where x = 2 or 4 in the case of R = H, CH3 and C6H5CH2, and x = 1 or 2 in the case of R = o-xylyl. The electrochem. properties of organofullerenes depend upon factors such as temperature and solvent as well as upon the number and type of addends. The near-IR absorption and ESR spectra of selected electroreduced (R)xC60 derivs. show similar ESR spectra which originate from at least two different types of radicals. The temperature dependence of the [(R)xC60]-spectra might be consistent with the formation of dimers.
- IT 172885-99-3 173006-79-6
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM
 (Formation, nonpreparative); RACT (Reactant or reagent)

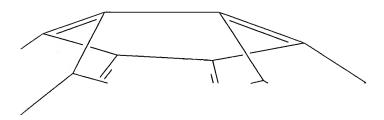


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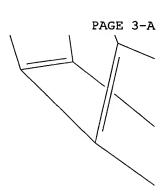


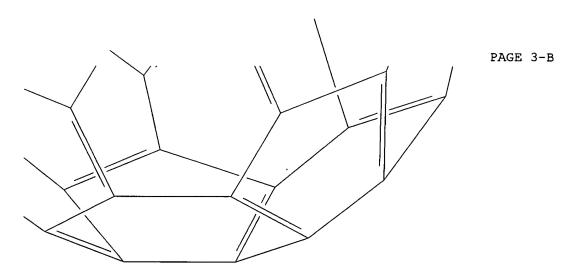


RN 173006-79-6 CAPLUS
CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)-, radical ion(2-) (9CI) (CA INDEX NAME)



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
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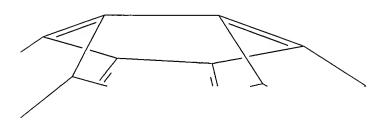


IT 172885-95-9

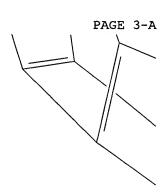
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (electrochem. reduction in various solvents)

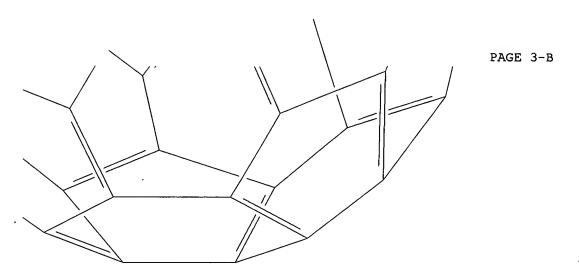
RN 172885-95-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
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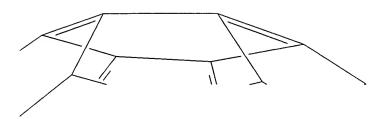
IT 173006-81-0

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

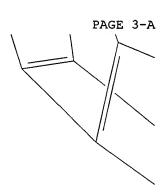
(electrochem. reductive formation and half-wave potential of)

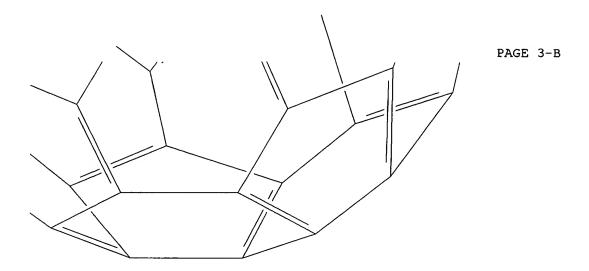
RN 173006-81-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)-, radical ion(3-) (9CI) (CA INDEX NAME)



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
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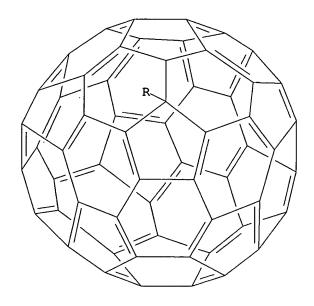


- L5 ANSWER 31 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:899337 CAPLUS
- DN 123:313538
- TI Cyanodihydrofullerenes and Dicyanodihydrofullerene: The First Polar Solid Based on C60
- AU Keshavarz-K, Majid; Knight, Brian; Srdanov, Gordana; Wudl, Fred
- CS Institute for Polymers and Organic Solids, University of California, Santa Barbara, CA, 93106-5090, USA
- SO Journal of the American Chemical Society (1995), 117(45), 11371-2
 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 123:313538
- AB The authors describe the synthesis of 1-cyano-2-protio dihydrofullerene (2), 1-cyano-2-Me dihydrofullerene (3), 1-cyano-2-p-tert-butylbenzyl dihydrofullerene (4), and 1,2-dicyano dihydrofullerene (5). The 1st crystal structural of any dihydrofullerene, in this case 5, is described. Surprisingly, it forms a polar solid with the nitrile dipoles pointing along the crystallog. b axis and also, the sp3 hybridized carbon atoms have very nearly tetrahedral angles (108.8°). 5 Has a 1st reduction wave 120 mV more pos. than C60.
- IT 170244-42-5P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and electrochem. reduction)
- RN 170244-42-5 CAPLUS
- CN [5,6]Fullerene-C60-Ih-1(9H)-carbonitrile, 9-[[4-(1,1-dimethylethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- L5 ANSWER 32 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:733939 CAPLUS
- DN 123:339357
- TI Isomerically pure organo[60] fullerenes from C602- salt: synthesis and characterization of 1-benzyl-2-hydro[60] fullerene

- ΑU Chen, Jian; Cai, Rui-Fang; Huang, Zu-En; Wu, Hou-Ming; Jiang, Shao-Kai; Shao, Qian-Fen
- CS Dep. Chem., Fudan Univ., Shanghai, 200433, Peop. Rep. China
- SO Journal of the Chemical Society, Chemical Communications (1995), (15), 1553-4CODEN: JCCCAT; ISSN: 0022-4936

- PB Royal Society of Chemistry
- Journal DT
- English LΑ
- CASREACT 123:339357 OS
- AB Isomerically pure 1-benzyl-2-hydro[60] fullerene is synthesized in 64% yield by the reaction of C602- potassium salt with benzyl chloride in THF at 50°C.
- IT 170646-75-0P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and characterization of 1-benzyl-2-hydro[60]fullerene)
- RN 170646-75-0 CAPLUS
- [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX CN NAME)





PAGE 2-A



- L5 ANSWER 33 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:713519 CAPLUS
- DN 123:313537
- Photolysis of o-methylbenzophenone in the presence of C60. Facile cleavage TI of the C-C bond connected to C60
- Tomioka, Hideo; Ichihashi, Masaki; Yamamoto, Katsutoshi AU
- CS Chemistry Dep. Materials, Mie Univ., Mie, 514, Japan

- 10/721,318 (RCE) Tetrahedron Letters (1995), 36(30), 5371-4 CODEN: TELEAY; ISSN: 0040-4039 PB Elsevier DΤ Journal LΑ English os CASREACT 123:313537 For diagram(s), see printed CA Issue. GI Irradiation of the title ketone with C60 gave 61-hydroxy-61-phenyl-1,9-AB (methano[1,2]benzenomethano)fullerene (I)(A = 6,6 bond substituted fullerene C60 moiety) as a result of Diels-Alder addition of 7-hydroxy-7-phenyl-o-quinodimethane with C60: the adduct is shown to undergo facile cleavage of the C-C bond connected to C60 either by silica gel chromatog. or upon heating in toluene to produce 1-(2benzoylphenyl)methyl-1,2-dihydrofullerene (II). IT 169964-19-6P RL: SPN (Synthetic preparation); PREP (Preparation) (photolysis of o-methylbenzophenone in the presence of C60, and facile cleavage of the C-C bond connected to C60) RN 169964-19-6 CAPLUS CN Methanone, [2-([5,6]fulleren-C60-Ih-1(9H)-ylmethyl)phenyl]phenyl- (9CI) (CA INDEX NAME) *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** L5 ANSWER 34 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN AN 1995:192398 CAPLUS DN 122:91357 TT Reversible reduction potentials of some new organofullerenes ΑU Evans, Dennis H.; Lerke, Susan A. Department Chemistry and Biochemistry, University Delaware, Newark, DE, CS 19716, USA SO Proceedings - Electrochemical Society (1994), 94-24 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 1087-97 CODEN: PESODO; ISSN: 0161-6374 DTJournal English LΑ AΒ Reversible potentials for the 1st 3 steps of reduction of 1,2-xylenediyl-, 1-methyl-4-t-butyl-and 1-benzyl-4-t-butyl-C60 in THF are reported. Each potential for these compds. is shifted .apprx.0.1 V in the neg. direction compared to the corresponding potentials of the parent fullerene. Published data for related compds. are reviewed, and the results are discussed in relation to those obtained with aromatic hydrocarbon analogs. IT **160482-48-4**, 1-Benzyl-4-t-butylfullerene(C60) RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

(reversible reduction potentials of new organofullerenes)

(Reactant); PROC (Process); RACT (Reactant or reagent)

RN

CN

(9CI)

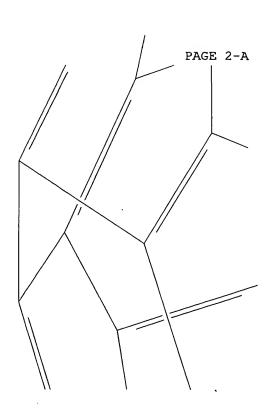
160482-48-4 CAPLUS

(CA INDEX NAME)

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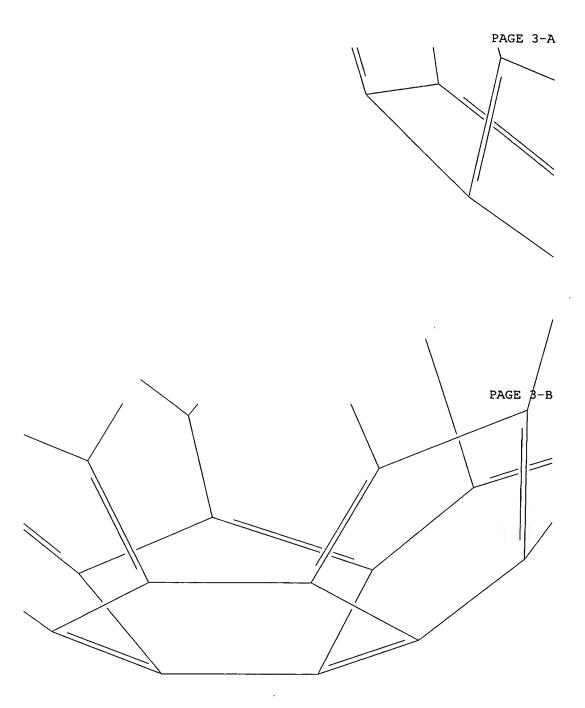
[5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-



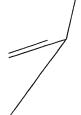


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PAGE 3-C



- L5 ANSWER 35 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1994:482375 CAPLUS
- DN 121:82375
- TI Addition of alkyl radicals to C60. Part 3. The EPR spectra of R3C60 radicals and a theoretical study of HC60 and H3C60 radicals
- AU Morton, J. R.; Negri, F.; Preston, K. F.
- CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A OR6, Can.
- SO Canadian Journal of Chemistry (1994), 72(3), 776-82 CODEN: CJCHAG; ISSN: 0008-4042
- DT Journal
- LA English
- AB The EPR spectra of a series of C60 adducts of the type R3C60 are described and discussed. In every case, two of the three ligands are equivalent, leading to the conclusion that the R3C60 radicals have a plane of symmetry. The unpaired electron distributions in mono- and trisubstituted-C60 radicals are computed with the help of the QCFF/PI and MNDO Hamiltonians. It is shown that the hyperfine consts. predicted on the basis of the calculated spin densities reproduce well the values observed

and

- suggest a reassignment of framework 13C coupling consts. in RC60.
- IT 140700-29-4P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and ESR spectrum of)
- RN 140700-29-4 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-(9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

- L5 ANSWER 36 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1994:234435 CAPLUS
- DN 120:234435
- TI ESR hyperfine patterns for the radicals derived from C60 and C70
- AU Balasubramanian, K.
- CS Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA
- SO Chemical Physics Letters (1993), 210(1-3), 153-8 CODEN: CHPLBC; ISSN: 0009-2614
- DT Journal
- LA English
- AB Theor. ESR hyperfine patterns for the radicals derived from C60 and C70 fullerenes are obtained from combinatorial techniques based on the group-theor. generating functions. Computerized combinatorial methods are

used to obtain simulated ESR hyperfine patterns. The ESR hyperfine patterns for several RnC60 radicals are obtained and compared with experiment 150733-25-8 154362-77-3

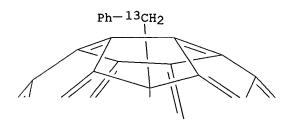
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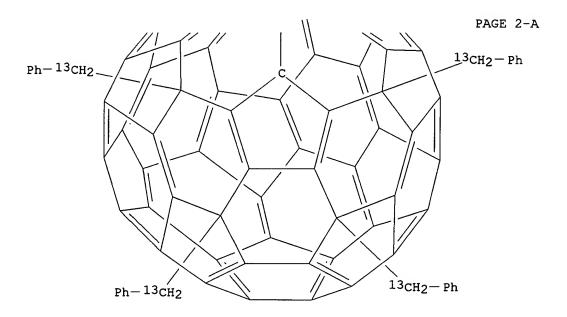
(ESR hyperfine pattern of)

RN 150733-25-8 CAPLUS

ΙT

CN [5,6]Fulleren-C60-Ih-1(9H)-yl, 6,9,12,15,18-pentakis(phenylmethyl-13C3)-(9CI) (CA INDEX NAME)





RN 154362-77-3 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl-13C)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

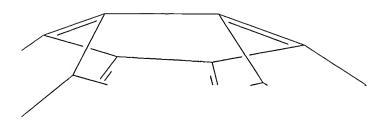
- L5 ANSWER 37 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1993:147000 CAPLUS
- DN 118:147000
- TI Radical adducts of fullerenes C60 and C70 studied by laser flash photolysis and pulse radiolysis
- AU Dimitrijevic, Nada M.; Kamat, Prashant V.; Fessenden, Richard W.
- CS Radiat. Lab., Univ. Notre Dame, Noret Dame, IN, 46556, USA
- SO Journal of Physical Chemistry (1993), 97(3), 615-18 CODEN: JPCHAX; ISSN: 0022-3654
- DT Journal
- LA English
- AB The reaction of R• (I; R = PhCH2, Me3C, Cl3C, Cl2CH) with C60 and C70 was examined using laser flash photolysis and pulse radiolysis. The alkyl radicals are very reactive toward fullerenes and form radical adducts, (RC60)• and (RC70)•. The difference absorption spectrum of (RC60)• exhibits broad absorption in the visible; that of (RC70)• exhibits bleaching of absorption in the region 440-560 nm. The rate consts. for the reaction of these radicals with fullerenes are in the range of 108 M-1 s-1 for I (R = Cl2CH) to diffusion controlled for I (R = Me3C).
- IT 140656-83-3

RL: PRP (Properties)

(UV of)

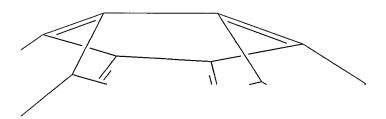
- RN 140656-83-3 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

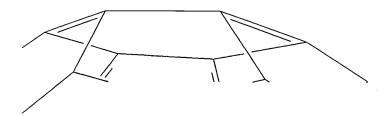


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- L5 ANSWER 38 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1993:59182 CAPLUS
- DN 118:59182
- TI Electron paramagnetic resonance spectra of fullerene R-C60 radicals. Evidence for RC60C60R dimers
- AU Morton, J. R.; Preston, K. F.; Krusic, P. J.; Wasserman, E.
- CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A OR9, Can.
- SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1992), (9), 1425-9 CODEN: JCPKBH; ISSN: 0300-9580
- DT Journal
- LA English
- Alkyl radicals generated in solution by UV photolysis add to C60 to form adducts of the type RC60, whose EPR spectra are discussed. When R = CCl3, CBr3, tert-Bu or 1-adamantyl, the spectrum is sufficiently powerful to permit the detection of several 13C satellites associated with the C60 component of the free radical. It is concluded from the intensities and hyperfine interactions of these satellites that ca. 2/3 of the unpaired spin population is located on the three carbon atoms ortho to that bearing the incoming radical R. There is evidence from the temperature dependence of the EPR spectra of certain RC60 radicals that they exist in equilibrium with their dimer, RC60C60R. For R = iso-Pr, tert-Bu, 1-adamantyl and CCl3, the enthalpy of dissociation is 35.5, 22.0, 21.6 and 17.1 kcal mol-1 resp.
- IT 140656-83-3P 140656-84-4P 140656-85-5P
 RL: PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation)
 (formation and ESR of)
- RN 140656-83-3 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * RN 140656-84-4 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl-13C)- (9CI) (CA INDEX NAME)



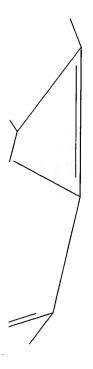
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * RN 140656-85-5 CAPLUS
 CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenyl-d5-methyl)- (9CI) (CA INDEX NAME)
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 1-C



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 2-C



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 3-C

- L5 ANSWER 39 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1992:204227 CAPLUS
- DN 116:204227
- TI ESR studies of the reaction of alkyl radicals with fullerene (C60)
- AU Morton, J. R.; Preston, K. F.; Krusic, P. J.; Hill, S. A.; Wasserman, E.
- CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A OR9, Can.
- SO Journal of Physical Chemistry (1992), 96(9), 3576-8 CODEN: JPCHAX; ISSN: 0022-3654
- DT Journal
- LA English
- AB Photolytically and thermally generated alkyl radicals (R• = tert-Bu, 1-adamantyl, iso-Pr, Et, and benzyl) react with C60 to form R-C60• radical adducts which were identified by the proton and 13C hyperfine interactions obtained from their ESR spectra. Consideration of the 13C spectra shows that the unpaired electron in R-C60• is mostly confined to 2 fused, 6-membered rings on the C60 surface, having the substituent R

at one of the points of fusion. Each half of the resulting radical structure of Cs symmetry can be compared with a cyclohexadienyl radical. Extensive delocalization of the unpaired electron over he C60 sphere is ruled out.

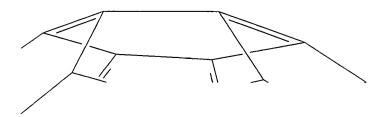
IT 140656-83-3P 140656-84-4P 140656-85-5P

RL: PRP (Properties); PREP (Preparation)

(formation and ESR spectrum of, from reaction of fullerene with photolytically or thermally generated alkyl radicals)

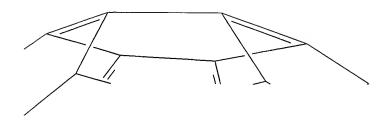
RN 140656-83-3 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * RN 140656-84-4 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl-13C)- (9CI) (CA INDEX NAME)

PAGE 1-A



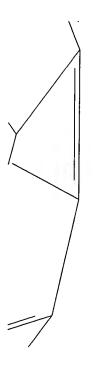
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * RN 140656-85-5 CAPLUS
- CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenyl-d5-methyl)- (9CI) (CA INDEX NAME)
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 1-C



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 2-C



- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

PAGE 3-C

- L5 ANSWER 40 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1992:193587 CAPLUS
- DN 116:193587
- TI Radical reactions of C60
- AU Krusic, P. J.; Wasserman, E.; Keizer, P. N.; Morton, J. R.; Preston, K. F.
- CS E. I. du Pont de Nemours and Co., Wilmington, DE, 19880-0328, USA
- SO Science (Washington, DC, United States) (1991), 254(5035), 1183-5
 - CODEN: SCIEAS; ISSN: 0036-8075
- DT Journal
- LA English
- AB Photochem. generated benzyl radicals react with C60 producing radical and nonradical adducts RnC60 (R = C6H5CH2) with n = 1 to at least 15. The radical adducts with n = 3 and 5 are stable above 50° and have been identified by ESR spectroscopy as the allylic R3C60• and cyclopentadienyl R5C60· radicals. The unpaired electrons are highly localized on the C60 surface. The extraordinary stability of these

radicals can be attributed to the steric protection of the surface radical sites by the surrounding benzylsubstituents. Photochem. generated Me radicals also add readily C60. Mass spectrometric analyses show the formation of (CH3)nC60 with n=1 to at least 34.

IT 140700-29-4P

RL: PREP (Preparation)

(allylic, formation and ESR of)

RN 140700-29-4 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-(9CI) (CA INDEX NAME)

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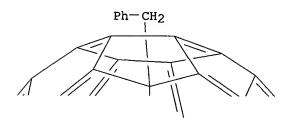
IT 139141-78-9P

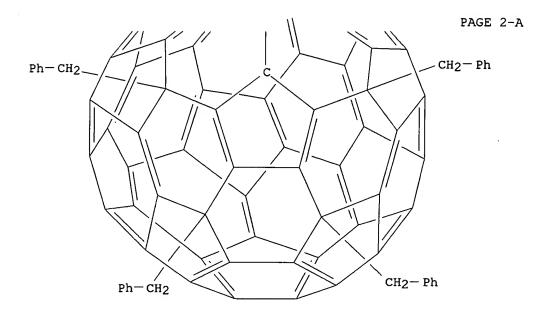
RL: PREP (Preparation)

(cyclopentadienyl, formation and ESR of)

RN 139141-78-9 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(9H)-yl, 6,12,15,18-tetrahydro-6,9,12,15,18-pentakis(phenylmethyl)- (9CI) (CA INDEX NAME)





=> s 14 not 15 L6 49 L4 NOT L5

=> dis 16 1-49 bib abs

L6 ANSWER 1 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:283633 CAPLUS

TI Titanium(III) Trisamidotriazacyclononane: Reactions with C60 and Radicals

AU Barroso, Sonia; Cui, Jinlan; Dias, Alberto R.; Duarte, M. Teresa; Ferreira, Humberto; Henriques, Rui T.; Oliveira, M. Conceicao; Ascenso, Jose R.; Martins, Ana M.

CS Centro de Quimica Estrutural, Instituto Superior Tecnico, Lisbon, 1049-001, Port.

SO Inorganic Chemistry (2006), 45(9), 3532-3537 CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

AB The reaction of titanium trisamidotriazacyclononane, [Ti{N(Ph)SiMe2}3tacn] (1), with C60 gave [Ti{N(Ph)SiMe2}3tacn]C60 (2) in high yield. Treatment of 2 with PhCH2Br gave [Ti{N(Ph)SiMe2}3tacn]Br and the radical PhCH2C60 (3). The reaction of CH3I with 1 gives two products. One is [Ti{N(Ph)SiMe2}3tacn]I (4), which results from the oxidation of 1 by an I radical. The other product, 5, resulting from a multistep reaction scheme that involves redox and nucleophilic reactions, presents an imido ligand formed by ligand rearrangement upon C-N bond cleavage. In solution, an exchange process that corresponds to a reversible 1,3-silyl shift between two Ti-bonded N atoms leads to isomers 5a and 5b. This equilibrium transforms an imido (TiNPh) into an amido ligand (Ti{NPh}SiMe2CH2Ph) with concomitant generation of an anionic moiety in the originally neutral triazacyclononane ring. In solution, either 5a or 5b displays addnl. fluxional processes that consist of its corresponding racemization processes.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
L6
AN
    2005:451357 CAPLUS
DN
    143:7512
ΤI
    A preparation of octahydrophenanthrenecarboxylic acid hydrazide
    derivatives, useful as glucocorticoid receptor modulators
IN
    Robinson, Ralph Pelton, Jr.; Kleinman, Edward Fox; Cheng, Hengmiao
PA
    Pfizer Products Inc., USA
SO
    PCT Int. Appl., 44 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                              DATE APPLICATION NO.
                      KIND
                                                               DATE
                                       _____
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                             _____
                                                              -----
                              20050526 WO 2004-IB3671
    WO 2005047254
PT
                       A1
                                                              20041108
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            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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NE, SN, TD, TG
PRAI US 2003-519937P P 20031113
OS MARPAT 143:7512

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a preparation of octahydrophenanthrenecarboxylic acid hydrazide derivs. of formula I [wherein: R1 is 1 to 6 independent substituents; R2 is 1 or 2 independent substituents selected from H, alkyl optionally substituted with 1-3 halogens, alkynyl, or OH, etc.; R3 is heterocycle], useful as glucocorticoid receptor modulators. The invention compds. are useful in the treatment of obesity, diabetes, anxiety, or inflammatory diseases. For instance, octahydrophenanthrenecarboxylic acid hydrazide derivative II was prepared from naphthalene derivative III in 9 steps.

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,

Preferred invention compds. showed ED50 less than 3 μM . RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2005:441043 CAPLUS
- DN 143:115583
- TI Syntheses, Structure, and Derivatization of Potassium Complexes of Penta(organo)[60]fullerene-Monoanion, -Dianion, and -Trianion into Hepta-and Octa(organo)fullerenes
- AU Matsuo, Yutaka; Nakamura, Eiichi

- CS Nakamura Functional Carbon Cluster Project ERATO, Japan Science and Technology Agency, Tokyo, 113-0033, Japan
- SO Journal of the American Chemical Society (2005), 127(23), 8457-8466 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 143:115583
- Two-electron reduction of penta(organo)[60]fullerenes C60Ar5H (Ar = Ph and AB biphenyl) by K/Hq amalgam afforded K complexes of the corresponding open-shell radical dianions [K+(THF)n]2[C60Ar52-•]. These compds. were characterized by UV-visible-near-IR and ESR spectroscopy in solution Anaerobic crystallization of [K+(THF)n]2[C60(biphenyl)52-◆] that exists largely as a monomer in solution gave black crystals of its dimer [K+(THF)3]4[(biphenyl)5C60-C60(biphenyl)54-], in which the two fullerene units are connected by a C-C single bond [1.577(11) Å] as determined by x-ray diffraction. Three-electron reduction of C60Ar5H with metallic K gave a black-green trianion [K+(THF)n]3[C60Ar53-]. The reaction of the trianion with an alkyl halide RBr (R = PhCH2 and Ph2CH) regioselectively afforded a hepta-organofullerene C60Ar5R2H, from which a K complex [K+(THF)n][C60(biphenyl)5(CH2Ph)2-] and a Pd complex $Pd[C60(biphenyl)5(CH2Ph)2](\pi-methallyl)$ as well as octa-organofullerene compds. C60(biphenyl)5(CH2Ph)3H2 and Ru[C60(biphenyl)5(CH2Ph)3H]Cp were synthesized. These compds. possess dibenzo-fused corannulene π -electron conjugated systems and are luminescent.
- RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 ANSWER 4 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
```

- AN 2005:99334 CAPLUS
- DN 142:170109
- TI Antiglucocorticoids for the treatment of catatonia
- IN Belanoff, Joseph K.
- PA Corcept Therapeutics, Inc., USA
- SO PCT Int. Appl., 28 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

	PATENT NO.					KIN	D	DATE			APPLICATION NO.						DATE			
PI		2005009388 2005009388				A2 A3		20050203		WO 2004-US23761						20040723				
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												JP,								
												MK,								
												SC,								
												UZ,								
		RW:																		
												BE,								
												LU,								
						BF,	BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,		
		SN, TD, TG																		
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	CA					AΑ											20040723			
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PRAI US 2003-489671P
                                  20030723
                           Ρ
     WO 2004-US23761
                           W
                                  20040723
AR
     The invention provides a method of ameliorating the symptoms of catatonia
     in a patient who is in need of treatment for catatonia. The method
     comprises administration of a therapeutically effective amount of a
     glucocorticoid receptor antagonist to the patient.
L6
     ANSWER 5 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:99329 CAPLUS
     142:170108
DN
ΤI
     Antiglucocorticoid therapy for the prevention of neurological damage in
     premature infants receiving glucocorticoid therapy
     Belanoff, Joseph K.
IN
PA
     Corcept Therapeutics, Inc., USA
SO
     PCT Int. Appl., 25 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
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                                                                       DATE
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     WO 2005009382
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             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-489601P
                           Р
                                 20030723
     WO 2004-US23592
                           W
                                 20040722
AB
     This invention pertains to the discovery that agents which inhibit the
     binding of cortisol to its receptors can be used in methods for preventing
     neurol. damage associated with glucocorticoid therapy in ventilator-dependent
     low birth weight preterm infants. Mifepristone, a potent glucocorticoid
     receptor antagonist, can be used in these methods.
     ANSWER 6 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:1013677 CAPLUS
     142:134293
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- L6
- AN
- DN
- Manganese(III) acetate-mediated free radical reactions of [60] fullerene ΤI with β -dicarbonyl compounds
- Li, Changzhi; Zhang, Danwei; Zhang, Xiaotong; Wu, Shihui; Gao, Xiang AU
- CS Department of Chemistry, Fudan University, Shanghai, 200433, Peop. Rep. China

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SO
      Organic & Biomolecular Chemistry (2004), 2(23), 3464-3469
      CODEN: OBCRAK; ISSN: 1477-0520
PB
      Royal Society of Chemistry
DT
      Journal
LΑ
      English
os
      CASREACT 142:134293
AB
      [60] Fullerene reacted with various \beta-dicarbonyl compds. in the
      presence of Mn(OAc)3.2H2O to generate dihydrofuran-fused
      [60] fullerene derivs. or 1,4-bisadducts. Dihydrofuran-fused [60] fullerene
      derivs. could be formed by treatment of \alpha-unsubstituted
      \beta-diketones or \beta-ketoesters with [60] fullerene in refluxing
      chlorobenzene in the presence of Mn(III). Solvent-participated unsym.
      1,4-bisadducts were obtained through the reaction of [60]fullerene with
     di-Me malonate or \alpha-substituted \beta-dicarbonyl compds. in
      toluene. A possible reaction mechanism for the formation of different
      fullerene derivs. is proposed.
RE.CNT 41
               THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 7 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
L6
     2004:681540 CAPLUS
ΑN
DN
     141:185588
ΤI
     Methods for the treatment of postpartum psychosis with glucocorticoid
     receptor antagonists
IN
     Belanoff, Joseph K.
     Corcept Therapeutics, Inc, USA
PA
SO
     PCT Int. Appl., 27 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
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                                                 APPLICATION NO.
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              MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
              GQ, GW, ML, MR, NE, SN, TD, TG
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     US 2004229855
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PRAI US 2003-445284P
                            P
                                    20030204
     WO 2004-US3183
                             W
                                    20040204
AB
     This invention generally pertains to the field of psychiatry. In
     particular, this invention pertains to the discovery that agents which
     inhibit the binding of cortisol to its receptors can be used in methods
     for treating postpartum psychosis. Mifepristone, a potent specific
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glucocorticoid receptor antagonist, can be used in these methods. The invention also provides a kit for treating postpartum psychosis in a human including a glucocorticoid receptor antagonist and instructional material

teaching the indications, dosage and schedule of administration of the glucocorticoid receptor antagonist.

- L6 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:450745 CAPLUS
- DN 141:23730
- TI Preparation of hydro(alkyl)fullerenes and their transition metal complexes, pentahydrofullarene transition metal complexes, and pentaalkylfullerenes
- IN Nakamura, Eiichi; Togano, Motoki
- PA Mitsubishi Chemical Corp., Japan
- SO Jpn. Kokai Tokkyo Koho, 22 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI	JP 2004155674 JP 2002-320701	A2	20040603 20021105	JP 2002-320701	20021105

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Hydro(alkyl)fullerenes CxRsH(5-s)H [I; Cx = fullerene skeleton; R = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl; x = even number

of ≥60; s = 0-4] are prepared by treatment of fullerenes or fullerene-organic compound adducts CxRp (II) or CxRpH (III) (Cx, R, x, s = same as above; p = 2, 4; q = 1, 3) with transition metal precursors and optional reducing agents in the presence of protonation agents. Hydroalkylfullerene transition metal complexes CxRmH(5-m)MLn (IV; Cx, R, x = same as I; M = transition metal; L = ligand; m = 1-4; n = 0-5) are prepared by treatment of II or III with transition metal precursors and optional reducing agents. Pentahydrofullerene transition metal complexes CxH5MLn (Cx, x = same as I; M, L, n = same as IV) are prepared by treatment of fullerenes with transition metal precursors and optional reducing agents. Pentaalkylfullerene metal complexes CxRmR'(5-m)MLn [V; Cx, x, R = same as I; R' = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl; M, L, m, n = same as IV] are prepared by treatment

of CxRmH(5-m)MLn (Cx, R, M, L, m, n = same as V) with R'X (R' same as V; X = leaving group). Thus, C60 fullerene was treated with [FeCp(CO)2]2 (Cp = η 5-cyclopentadienyl) to give 25% VI.

- L6 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:447092 CAPLUS
- DN 141:7284
- TI Preparation of hydro(alkyl)fullerenes and their transition metal complexes, and pentahydrofullerene transition metal complexes
- IN Nakamura, Eiichi; Togano, Motoki
- PA Mitsubishi Chemical Corp., Japan
- SO Jpn. Kokai Tokkyo Koho, 17 pp. CODEN: JKXXAF
- DT Patent

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Japanese
FAN.CNT 1
                                         APPLICATION NO.
    PATENT NO.
                      KIND
                              DATE
                                                              DATE
    JP 2004155675
                        A2
                              20040603
PΤ
                                         JP 2002-320702
                                                               20021105
PRAI JP 2002-320702
                              20021105
OS
    CASREACT 141:7284
GI
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Hydro(alkyl)fullerenes CxRpH(5-p)H [1; Cx = fullerene skeleton; R = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl; x = even number

of ≥ 60 ; p = 0-4] having partial structures II (A = H, R; R = same as 1; P = H), hydroalkylfullerene transition metal complexes CxRmH(5-m)MLn (3; Cx, R, x = same as 1; M = transition metal; L = $\eta 1$ - or $\eta 2$ -ligand; m = 1-4; n = 0-5) having partial structures IV (A = same as II; M, L, n = same as 3), and pentahydrofullerene transition metal complexes CxH5MLn (Cx, x = same as 1; M, L, n = same as 3) having partial structures V (M, L, n = same as 3) are prepared Thus, C60 fullerene having partial structure II (A = H, P = CH2Ph) was treated with 9,10-dihydroanthracene and Re2(CO)10 to give 42% C60 fullerene having partial structure IV (one of A = CH2Ph, others of A = H, M = Re, L = CO, n = 3).

- L6 ANSWER 10 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:412780 CAPLUS
- DN 140:400079
- TI Methods for treating gastroesophageal reflux disease with glucocorticoid receptor antagonists
- IN Belanoff, Joseph K.
- PA Corcept Therapeutics, Inc., USA
- SO PCT Int. Appl., 27 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN. CNT 2

21111	PATE	KIND DATE				APPL														
PI		2004041215 2004041215				A2 A3		20040521 20041104		1	WO 2	003-1		20031105						
	•	W:						AU,												
								DK,												
			GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,		
			LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NI,	NO,	NZ,		
			OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ТJ,	TM,		
			TN,	TR,	TT,	TZ,	UA,	ŪG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW				
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,		
			BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,		
			ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,		
			TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
	CA 2				AA				(CA 2003-2504751					20031105					
	AU 2	AU 2003291322				A1	A1 20040607				AU 2003-291322					20031105				
	US 2004132703					A 1		2004	0708	1	US 2003-703069					20031105				

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US 2004167110
                           A1
                                  20040826
                                             US 2003-702950
                                                                       20031105
     EP 1567167
                           A2
                                  20050831
                                             EP 2003-768714
                                                                       20031105
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2006507311
                           Т2
                                  20060302
                                              JP 2004-550523
                                                                       20031105
PRAI US 2002-424199P
                           Ρ
                                  20021105
     WO 2003-US35341
                           W
                                  20031105
AB
     This invention relates to the discovery that agents capable of inhibiting
     the biol. action of the glucocorticoid receptor can be used in methods for
     treating gastroesophageal reflux disease in a subject. The glucocorticoid
     receptor antagonist is especially mifepristone.
L6
     ANSWER 11 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2004:412779 CAPLUS
DN
     140:400109
     Methods using glucocorticoid receptor antagonists for treating migraine
ΤI
IN
     Belanoff, Joseph K.
PA
     Corcept Therapeutics, Inc., USA
so
     PCT Int. Appl., 30 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 2
                               DATE
                          KIND
                                            APPLICATION NO.
                                                                      DATE
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     WO 2004041214
                          A2
PΙ
                                 20040521 WO 2003-US35328
                                                                      20031105
     WO 2004041214
                          A3
                                 20041111
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                           CA 2003-2504697
     CA 2504697
                          AA
                                 20040521
                                                               20031105
     AU 2003291314
                          A1
                                 20040607
                                              AU 2003-291314
                                                                      20031105
                                              US 2003-703069
     US 2004132703
                          A1
                                 20040708
                                                                      20031105
     US 2004167110
                                 20040826
                          A1
                                              US 2003-702950
                                                                      20031105
     EP 1581234
                          A2
                                 20051005
                                           EP 2003-768706
                                                                      20031105
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2006508951
                          T2 20060316 JP 2004-550521
                                                                     20031105
     US 2006052354
                           A1
                                 20060309
                                              US 2005-533146
                                                                      20050427
PRAI US 2002-424199P
                          P
                                 20021105
     WO 2003-US35328
                          W
                                 20031105
AB
     The invention relates to the discovery that agents capable of inhibiting
     the biol. action of the glucocorticoid receptor can be used in methods for
     treating migraine in a subject.
L6
     ANSWER 12 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2004:383047 CAPLUS
DN
TI
     Discovery of potent, non-steroidal and highly selective glucocorticoid
     receptor antagonists with anti-obesity activity
AU
     Morgan, Bradley P.; Liu, Kevin K.-C.; Dalvie, Deepak K.; Swick, Andrew G.;
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- Hargrove, Diane M.; Wilson, Theresa C.; LaFlamme, Janet A.; Moynihan, Melinda S.; Rushing, Margaret A.; Woodworth, Graeme F.; Li, Jisong; Trilles, Richard V.; Yang, Xiaojing; Harper, Kenneth W.; Carroll, Richard S.; Martin, Kelly A.; Nardone, Nancy A.; O'Donnell, John P.; Faletto, Michael B.; Vage, Chandravathi; Soliman, Victor
- CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06340, USA
- SO Letters in Drug Design & Discovery (2004), 1(1), 1-5 CODEN: LDDDAW; ISSN: 1570-1808
- PB Bentham Science Publishers Ltd.
- DT Journal; General Review
- LA English
- AB A review. To thwart phase II metabolism, Structure-Activity-Relationship (SAR) studies around the phenol of the potent glucocorticoid receptor (GR) antagonists CP-394531 and CP-409069 were examined The discovery of the potent; selective, nonsteroidal GR antagonist (CP-472555) with anti-GR and anti-obesity activity in animal models is described.
- RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:274878 CAPLUS
- DN 141:54056
- TI Selective addition to [60] fullerene of two different radicals generated from Mn(III)-based radical reaction
- AU Wang, Guan-Wu; Zhang, Ting-Hu; Cheng, Xin; Wang, Fan
- CS Department of Chemistry, University of Science and Technology of China, Hefei, 230026, Peop. Rep. China
- SO Organic & Biomolecular Chemistry (2004), 2(8), 1160-1163 CODEN: OBCRAK; ISSN: 1477-0520
- PB Royal Society of Chemistry
- DT Journal
- LA English
- OS CASREACT 141:54056
- AB Reaction of [60] fullerene in PhMe with RCH(CO2Et)2 [R = Me, Et, Br] CH(CO2Et)3, and NCCH2CO2Et in the presence of Mn(OAc)3.2H2O afforded benzyl-substituted unsym. 1,4-adducts. Dibenzylated 1,4-adduct and a methanofullerene 6 were also obtained in the case of CH(CO2Et)3 and NCCH2CO2Et, resp. A possible reaction mechanism for the formation of the 1,4-adducts is proposed.
- RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:141753 CAPLUS
- DN 140:339056
- TI Methodology for the Preparation of C1-Monoalkylated 1,2-Dihydro[C70]
 Derivatives: Formation of the "Other" Regioisomer
- AU Wang, Zhongwen; Meier, Mark S.
- CS Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA
- SO Journal of Organic Chemistry (2004), 69(6), 2178-2180 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 140:339056
- AB Deprotonation of 1,2-C70H2 with Bu4N+ OH-, followed by alkylation with Me

bromoacetate, results in formation of a C(1)-monoalkylated 1,2-dihydro-C70 derivative The position of the alkyl group (C-1) was established by NMR spectroscopy and comparison with literature spectra of C(2)-monoalkylated analogs. Presumably, C(1)-alkylation is the major process due to selective deprotonation of 1,2-C70H2 at C-1. Substitution of benzyl bromide for Me bromoacetate results in rapid dialkylation, unless the amount of base is carefully controlled, in which case C(1)-monobenzylation is the major process. This methodol. for alkylation at C-1 is complimentary to methods for the C(2)-monoalkylation of C70 with Zn and Me bromoacetate.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 15 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
L6
AN
     2004:41424 CAPLUS
DN
     140:111136
     Preparation of octahydrophenanthrenols as glucocorticoid receptor
TT
     modulators for treatment of inflammatory conditions
     Chantigny, Yves Andre; Kleinman, Edward Fox; Robinson, Ralph Pelton, Jr.
IN
     Pfizer Products Inc., USA
PA
SO
     PCT Int. Appl., 143 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                           KIND
                                   DATE
                                                APPLICATION NO.
                                                                         DATE
                           ____
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ΡI
     WO 2004005229
                            A1
                                   20040115
                                                WO 2003-IB2941
                                                                         20030625
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2491994 AA 20040115 CA 2003-2491994 20030625 AU 2003281355 **A1** 20040123 AU 2003-281355 20030625 EP 1521733 **A1** 20050413 EP 2003-740911 20030625 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK BR 2003012575 Α 20050503 BR 2003-12575 20030625 JP 2005532389 T2 20051027 JP 2004-519100 20030625

US 2003-615126

20030708

US 2004138262 A1 20040715 PRAI US 2002-394425P P 20020708 WO 2003-IB2941 W 20030625

OS MARPAT 140:111136

GI

AΒ Title compds. I [wherein A = CR6R7CR8R9, COCR10R11, or CR12=CR13; X and Y = independently H, F, Cl, Br, or alkyl; R1 = alkyl, alkenyl, or (un) substituted benzyl; R2 = (un) substituted (cyclo) alkyl(alkyl), alkenyl, alkynyl, (hetero)aryl(alkyl), or heterocyclyl(alkyl); R3 = H or (un) substituted (cyclo) alkyl, alkenyl, alkynyl, heterocyclyl, or (hetero)aryl; R4 = OH or NR14R15; R5 = H, halo, OH, CN, or (un)substituted (cyclo)alkyl(oxy), alkenyl, alkynyl, (hetero)aryl(oxy), heterocyclyl(oxy), carbamoyl, sulfamoyl, acyl(oxy), etc.; R6-R9 = independently H, alkyl, F, or OH; R10 and R11 = independently H or alkyl; R12 and R13 = independently H, F, or alkyl; R14 and R15 = independently H or alkyl; and pharmaceutically acceptable salts thereof] were prepared as glucocorticoid receptor agonists (no data). For example, (3S, 4aR, 10aR)-3-bromo-4a-ethyl-7-hydroxy-3,4,4a,9,10,10a-hexahydro-1H-phenanthren-2-one (multi-step preparation given) was treated with NaOH in DMF and H2O followed by 0.2M HCl to give a 2:1 mixture of the 2-keto-3-hydroxy and 2-hydroxy-3-keto derivs. 2-keto enriched compound (9:1 ratio of 2-keto to 3-keto derivative) was alkylated with propyne in THF using BuLi in hexane to afford II (25%). Bioassays for glucocorticoid receptor modulation and antiinflammatory response are described, but no specific data are provided. Thus, I and their pharmaceutical compns., salts, and prodrugs are useful in the treatment of certain inflammatory disorders, endocrine disorders, collagen diseases, dermatol. diseases, allergic states, ophthalmic diseases, respiratory diseases, hematol. disorders, neoplastic diseases, edematous states, and gastrointestinal diseases (no data).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

II

L6 ANSWER 16 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:41222 CAPLUS

DN 140:87727

TI Methods using a glucocorticoid receptor antagonist for treating psychosis associated with interferon- α therapy

IN Belanoff, Joseph K.

PA Corcept Therapeutics, Inc., USA

SO PCT Int. Appl., 36 pp. CODEN: PIXXD2

DT Patent

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LA
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                       DATE
                          ____
                           A2
PΙ
     WO 2004004653
                                  20040115
                                              WO 2003-US21245
                                                                       20030702
     WO 2004004653
                           А3
                                  20040826
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
              PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2491296
                           AΑ
                                 20040115
                                             CA 2003-2491296
                                                                       20030702
     AU 2003269898
                           A1
                                 20040123
                                              AU 2003-269898
                                                                       20030702
     EP 1534299
                           A2
                                 20050601
                                              EP 2003-751785
                                                                       20030702
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     CN 1665515
                                 20050907
                           Α
                                             CN 2003-815811
                                                                       20030702
     JP 2005535664
                           T2
                                 20051124
                                              JP 2004-519990
                                                                       20030702
     US 2006063748
                                 20060323
                                              US 2004-519008
                           A1
                                                                       20041221
PRAI US 2002-393660P
                           Р
                                 20020702
     WO 2003-US21245
                           W
                                 20030702
     The invention discloses methods using a glucocorticoid receptor antagonist
AB
     for the treatment of psychosis associated with interferon-\alpha therapy.
     The invention further discloses kits for the treatment of Hepatitis C in a
     patient.
L6
     ANSWER 17 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2003:844743 CAPLUS
DN
     140:59737
     Synthesis of Ferrocene/Hydrofullerene Hybrid and Functionalized Bucky
ΤI
AU
     Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi
CS
     Department of Chemistry, The University of Tokyo, Bunkyo, Tokyo, 113-0033,
SO
     Journal of the American Chemical Society (2003), 125(46), 13974-13975
     CODEN: JACSAT; ISSN: 0002-7863
PB
     American Chemical Society
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- DT Journal
- LA English
- OS CASREACT 140:59737
- AB Hydroferration reaction of [60] fullerene or its derivs., C60(CH2Ph)2 and C60(CH2Ph)2PhH, with [Fe(C5H5)(CO)2]2 gives regionelectively a ferrocene/hydrofullerene hybrid, which upon treatment with Bu4NOH and an alkyl halide affords the corresponding alkylated bucky ferrocene, e.g., Fe(C60H5)(C5H5), again regionelectivity via an anion of the ferrocene. These alkylation conditions were applied to the rhenium analog to afford, e.g., Re[C60(CH2Ph)4Ph](CO)3 in 48% yield..
- RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:827349 CAPLUS
- DN 140:59751

- TI Synthesis and catalytic activity of rhodium diene complexes bearing indenyl-type fullerene $\eta 5$ -ligand
- AU Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi
- CS Department of Chemistry, The University of Tokyo, Hongo, Tokyo, 7-3-1, Japan
- SO Journal of Organometallic Chemistry (2003), 683(2), 295-300 CODEN: JORCAI; ISSN: 0022-328X
- PB Elsevier Science B.V.
- DT Journal
- LA English
- OS CASREACT 140:59751
- AB Rh n5-complexes bearing an indenyl-type fullerene ligand, Rh[C60(PhCH2)2Ph](cod) (2), Rh[C60(PhCH2)2Ph](nbd) (3) and Rh(C70Ph3)(cod) (4), were synthesized from the corresponding fullerene tri-adducts in 93-96% yields. X-ray crystallog. anal. of 4 indicated that the structure of 4 is similar to that of Rh(Ind)(cod). The Rh complex 2 catalyzes alkyne trimerization reactions and hydroboration reactions.
- RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:683501 CAPLUS
- DN 140:128146
- TI Mixed bis-functionalization of fullerene C60 from C602- anion
- AU Cheng, Fuyong; Allard, Emmanuel; Chopin, Stephanie; Delaunay, Jacques; Cousseau, Jack
- CS Laboratoire d'Ingenierie Moleculaire et Materiaux Organiques, UMR CNRS 6501, Universite d'Angers, Angers, 49045, Fr.
- SO Proceedings Electrochemical Society (2002), 2002-12(Fullerenes--Volume 12: The Exciting World of Nanocages and Nanotubes), 188-192 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- OS CASREACT 140:128146
- AB Mixed adducts bis-functionalization of fullerene can be derived from C602anion. In particular functionalized dihydrofullerenes C60HR are thus obtained, and can be used for obtaining various bis-functionalization of fullerene derivs.
- RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:655961 CAPLUS
- DN 139:323635
- TI Rhenium-templated regioselective polyhydrogenation reaction of [60]fullerene
- AU Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi
- CS Department of Chemistry, The University of Tokyo, Tokyo, 113-0033, Japan
- SO Angewandte Chemie, International Edition (2003), 42(30), 3530-3532 CODEN: ACIEF5; ISSN: 1433-7851
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- OS CASREACT 139:323635
- AB Rhenium-templated transfer hydrogenation from 9,10-dihydroanthracene (DHA) to [60] fullerene or its derivs. in water at 160° gave a 60% yield of cyclopentadiene-incorporated fullerene analog, e.g.,

C60(H)3(PhCH2)2(Ph) (2), which can be converted into the corresponding metal complexes. E.g., 2 reacts with {Fe(C5H5)(CO)2}2/PhCN at 160° to give a 28% yield of (C5H5)Fe[C60(H)3(PhCH2)2(Ph)].

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:610236 CAPLUS
- DN 139:154927
- TI Pharmaceutical compositions of amorphous dispersions of drugs and lipophilic microphase-forming materials
- IN Perlman, Michael Ellis; Shanker, Ravi Mysore; Babcock, Walter Christian; Friesen, Dwayne Thomas; Rabenstein, Mark David; Smithey, Daniel Tod
- PA Pfizer Products Inc., USA
- SO PCT Int. Appl., 89 pp.

CODEN: PIXXD2

- DT Patent
- LA English
- FAN.CNT 1

	PATENT NO.			KIND DATE			APPLICATION NO.					DATE						
ΡI	WO	2003	0638	33		A1	_	2003	0807							2	0030	128
		W:	ΑE,	AG,	AL,	AM,			ΑZ,									
									DM,									
									IS,									
									MG,									
									SE,									
									ZA,								·	
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
									ΑT,									
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
	CA	2474	838			AA		2003	0807		CA 2	003-	2474	838		2	0030	128
	EΡ	1469	832			A1		2004	1027		EP 2	003-	7004	35		2	0030	128
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
	BR	2003	0073	44		Α		2004	1214		BR 2	003	7344			2	0030	128
	JP	2005	5232	62		Т2		2005	0804		JP 2	003-	56352	27		20	0030	128
	US	2003	2283	58		A1		2003	1211	1	US 2	003-3	3557	47		20	0030	131
PRAI	US	2002	-354					2002	0201									
	WO	2003	-IB3	35		W		2003	0128									

AB A pharmaceutical composition comprises a solid amorphous dispersion comprising a low-solubility drug and a concentration-enhancing polymer and a lipophilic microphase-forming material. Alternatively, a solid amorphous dispersion comprising a low-solubility drug and a concentration-enhancing polymer is co-administered with a lipophilic microphase-forming material to an in vivo use environment. A spray solution was formed containing 2.5 wt% drug, 7.5 wt% HPMCAS-MF, and 90% acetone. The solution was spray-dried by directing a 2-fluid external-mix spray nozzle at 2.7 bar with a feed rate of 190 g/min into the stainless-steel chamber of a spray-dryer, by using nitrogen as the drying gas, maintained at a temperature of 137° at the inlet; the drying gas and evaporated solvent exited the drier at 49°. The resulting solid amorphous dispersion was collected and then dried in a solvent tray-drier by spreading the spray-dried particles onto polyethylene-lined trays to a depth of not more than 1 cm and then drying them at 40° for 25 h. After drying, dispersion 1 contained 25 wt% drug.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:534830 CAPLUS
- DN 140:59390
- TI Regioselective synthesis of [60] fullerene η 5-indenide R3C60- and η 5-cyclopentadienide R5C60- bearing different R groups
- AU Toganoh, Motoki; Suzuki, Kazuhiro; Udagawa, Rie; Hirai, Atsushi; Sawamura, Masaya; Nakamura, Eiichi
- CS Department of Chemistry, The University of Tokyo, Bunkyo-ku, Japan
- SO Organic & Biomolecular Chemistry (2003), 1(14), 2604-2611 CODEN: OBCRAK; ISSN: 1477-0520
- PB Royal Society of Chemistry
- DT Journal
- LA English
- OS CASREACT 140:59390
- AB Treatment of a 1,7-diorgano[60] fullerene with Grignard reagents or organocopper reagents affords a [60] fullerene indenide or a [60] fullerene cyclopentadienide regioselectively in good to excellent yields. These reactions gave an insight into the reaction mechanism of the organocopper penta-addition reaction of [60] fullerene, giving [60] fullerene cyclopentadienide in quant. yield.
- RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:531546 CAPLUS
- DN 139:108747
- TI Fullerene-containing dye and application such as optical recording materials, color composition for color filter, ink thereof
- IN Saito, Yasunori; Tsukahara, Hiroshi; Ogiso, Akira; Misawa, Tsutayoshi
- PA Mitsui Chemicals, Inc., Japan; Yamamoto Chemicals Inc.
- SO Jpn. Kokai Tokkyo Koho, 41 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese
- FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2003196881	A2	20030711	JP 2002-256809	20020902
PRAI	JP 2001-265981	Α	20010903		

- AB The invention relates to a fullerene dye disposed in an organic dye layer as an optical recoding layer on a substrate. The dye provides the good recording/reading characteristic using 300-500 nm light.
- L6 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:394587 CAPLUS
- DN 139:117205
- TI C602- Chemistry: C60 Adducts Bearing Two Ester, Carbonyl, or Alcohol Groups
- AU Allard, Emmanuel; Delaunay, Jacques; Cousseau, Jack
- CS Laboratoire D'Ingenierie Moleculaire et Materiaux Organiques, UMR CNRS 6501, Universite d'Angers, Angers, F-49045, Fr.
- SO Organic Letters (2003), 5(13), 2239-2242 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- LA English

- OS CASREACT 139:117205
- AB Reactions of activated halo compds. XCH2-A (X = Br, I; A = ester, ketone) with C602- anion give rise to C60(CH2-A)2 adducts (major products) along with unexpected methanofullerenes C60>CH-A and monosubstituted dihydrofullerenes C60(H)(CH2-A) (minor products). Methanofullerenes come from side reactions with X2CH-A traces.
- RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:318751 CAPLUS
- DN 139:164611
- TI New, scalable route for the synthesis of a trans-fused hexahydro-1H-phenanthren-2-one from a conjugated tetrahydro-3H-phenanthren-2-one
- AU Morgan, Bradley P.; Trilles, Richard V.; Woodworth, Graeme F.
- CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06371, USA
- SO Synthetic Communications (2003), 33(6), 915-920 CODEN: SYNCAV; ISSN: 0039-7911
- PB Marcel Dekker, Inc.
- DT Journal
- LA English
- OS CASREACT 139:164611
- AB A three-step, readily scalable route for the conversion of a ring-conjugated tetrahydro-3H-phenanthren-2-one to a trans-fused hexahydro-1H-phenanthren-2-one is described. The key step is the hydrogenation of a double bond using a nearby ketal moiety to assist in the stereoselective delivery of the hydrogen.
- RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:235760 CAPLUS
- DN 138:385156
- TI Monoalkylation of C60 and C70 with Zn and Active Alkyl Bromides
- AU Wang, Zhongwen; Meier, Mark S.
- CS Center for Advanced Carbon Materials and Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA
- SO Journal of Organic Chemistry (2003), 68(8), 3043-3048 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 138:385156
- AB A convenient and simple solution-phase electron-transfer reaction of C60 with zinc and α-bromoacetonitrile, α-bromoacetates, allyl bromide, benzyl bromide and α-bromo ketones in DMF gives different types of monoalkylated C60 derivs. When this method is employed with C70, 2-carbomethoxymethyl-1,2-dihydro[70] fullerene is produced as one of the two 1,2-monoalkylated C70 isomers, together with the first 5,6-monoalkylated C70 derivative
- RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:202422 CAPLUS
- DN 138:232194

- TI Methods for inhibiting cognitive deterioration in adults with Down's syndrome with glucocorticoid receptor blockade
- IN Belanoff, Joseph K.
- PA Corcept Therapeutics, Inc., USA
- SO PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FAN. CNT I																			
		PA.	CENT 1	NO.			KIN	D									DATE		
	ΡI	WO	2003	0202:	16		A1 20030313			WO 2002-US27576						20020827			
										AZ,									
				-	-		-	-	-	DM,		-			-			•	•
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			DET.	•	•	•		•	•	YU,	•		ma	116	736	0.52	2.00	22	20
			RW:							SD,									
										ES,								-	
								BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,
				•	•	TD,													
		CA	2459	033			AA		2003	0313	(CA 2	002-2	2459	033		2	0020	827
		EΡ	1432	379			A1		2004	0630]	EP 2	002-	7704	41		2	0020	827
			R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
				IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	SK		
		CN	1556	708			Α		2004	1222	(CN 2	002-	8186	80		2	0020	827
		JΡ	2005	50188	32		Т2		2005	0120		JP 2	003-	5245	30		2	0020	827
			2003						2003	0403	τ	JS 20	002-2	2305	75		2	0020	828
		ZA	2004	00175	54		Α			0303								0040	
			2004							0528								0040	
	PRAI								2001		•						_	0010.	
			2002				W		2002										
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- AB This invention generally pertains to the field of psychiatry. In particular, this invention pertains to the discovery that agents capable of inhibiting the binding of cortisol to its receptors can be used in methods for preventing or reversing cognitive deterioration in adults with Down's syndrome. Mifepristone, a potent specific glucocorticoid receptor antagonist, can be used in these methods. The invention also provides a kit for preventing or reversing cognitive deterioration in a DS patient including a glucocorticoid receptor antagonist and instructional material teaching the indications, dosage and schedule of administration of the glucocorticoid receptor antagonist.
- RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:49356 CAPLUS
- DN 139:85110
- TI Easy access to unprecedented mixed functionalized dihydrofullerenes C60RH and C60RR': the C602- anion route
- AU Allard, Emmanuel; Cheng, Fuyong; Chopin, Stephanie; Delaunay, Jacques; Rondeau, David; Cousseau, Jack
- CS Laboratoire IMMO (CNRS UMR 6501), Faculte des Sciences, Universite d'Angers, Angers, F-49045, Fr.
- SO New Journal of Chemistry (2003), 27(2), 188-192 CODEN: NJCHE5; ISSN: 1144-0546
- PB Royal Society of Chemistry

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DT Journal
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AB Functionalized mixed dihydrofullerenes C60RH and C60RR' are easily obtained from reactions between C602- anion and halo derivs. RX and R'X. The key step consists of the selective reaction of the intermediate [C60R]- ion, as soon as it is formed, with either CF3CO2H or R'X. This process is made possible thanks to the very fast single electron transfer reaction between C602- and RX. Functionalized dihydrofullerenes C60RH thus prepared are also shown to be very good starting compds. for obtaining various C60RR' derivs.

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
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AN 2003:5750 CAPLUS

DN 138:78446

TI Pharmaceutical compositions containing polymer and drug assemblies

IN Babcock, Walter Christian; Crew, Marshall David; Friesen, Dwayne Thomas; Rabenstein, Mark David; Smithey, Daniel Tod; Shanker, Ravi Mysore

PA Pfizer Products Inc., USA

SO PCT Int. Appl., 257 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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PATENT NO.
                           KIND
                                    DATE
                                                 APPLICATION NO.
                                                                           DATE
                            ____
                                    _____
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     WO 2003000226
                            A2
PI
                                    20030103
                                                 WO 2002-IB2256
                                                                           20020617
     WO 2003000226
                            A3
                                    20031023
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
              PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
              UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
              KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
              GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
              GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2450748
                            AΑ
                                    20030103
                                                 CA 2002-2450748
                                                                           20020617
     US 2003170309
                             A1
                                    20030911
                                                 US 2002-173945
                                                                           20020617
     EP 1401399
                            A2
                                    20040331
                                                 EP 2002-735849
                                                                           20020617
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002011028
                                    20040615
                                                BR 2002-11028
                            Α
                                                                           20020617
     JP 2004534811
                             T2
                                    20041118
                                                 JP 2003-506873
                                                                           20020617
PRAI US 2001-300259P
                            Р
                                    20010622
     WO 2002-IB2256
                            W
                                    20020617
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AB Solns. containing polymer/drug assemblies of a low-solubility drug and an amphiphilic polymer are disclosed. In addition, solid aggregated polymer/drug assemblies are disclosed comprising a low-solubility drug and polymer. For example, amorphous solid dispersions of the low-solubility drug 5-chloro-1H-indole-2-carboxylic acid [(1S)-benzyl-3-((3R,4S)-dihydroxypyrroldin-1-yl-)-(2R)-hydroxy-3-oxypropyl]amide and the amphiphilic polymer hydroxypropyl Me cellulose acetate succinate were prepared When no drug was present, small particles about 10-20 nm in size were present due to aggregation of the polymer (HPMCAS-MF) with itself,

LA English

OS CASREACT 139:85110

likely as a result of its amphiphilicity, which renders the polymer only sparingly water soluble For solns. containing drug solid dispersions, particles

were present with an average size of about 80 nm. This demonstrates the formation of polymer/drug assemblies in solution

- L6 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:524034 CAPLUS
- DN 137:232437
- TI Alkylation of Dihydrofullerenes
- AU Meier, Mark S.; Bergosh, Robert G.; Gallagher, Megan E.; Spielmann, H. Peter; Wang, Zhongwen
- CS Center for Advanced Carbon Materials and Department of Chemistry and Department of Molecular and Cellular Biochemistry, University of Kentucky, Lexington, KY, 40506-0055, USA
- SO Journal of Organic Chemistry (2002), 67(17), 5946-5952 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 137:232437
- The fulleride dianions C602- and C702- were generated by deprotonation of the hydrogenated fullerenes, 1,2-C60H2 and 1,2-C70H2. These anions were prepared in the presence of a variety of alkylating agents and mono- or dialkylated products were obtained. Alkylation was not successful with sulfonate ester alkylating agents. Deprotonation of monoalkylated compds., followed by a second alkylation with a different alkylating agent, produced heterodialkylated compds. The monoalkylated material was invariably the 1,2-isomers, while the dialkylated materials were generally 1,4-isomers, although some 1,2-isomer was observed in the C70 product. The major product from alkylation of C702- was the 7,23-isomer, a structure where the alkylation took place near the equator of the fullerene cage, rather than at the more strained carbons near the poles.
- RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:348359 CAPLUS
- DN 137:88411
- TI Discovery of Potent, Nonsteroidal, and Highly Selective Glucocorticoid Receptor Antagonists
- AU Morgan, Bradley P.; Swick, Andrew G.; Hargrove, Diane M.; LaFlamme, Janet A.; Moynihan, Melinda S.; Carroll, Richard S.; Martin, Kelly A.; Lee, Eunsun; Decosta, Debra; Bordner, Jon
- CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06371,
- SO Journal of Medicinal Chemistry (2002), 45(12), 2417-2424 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- AB An approach to the computer-assisted, pharmacophore design of nonsteroidal templates for the glucocorticoid receptor (GR) that contained an element of pseudo-C2 symmetry was developed. The enantiomer of the initial design, and not the designed mol., showed the desired ligand binding to the GR. The pseudo-C2 symmetry of the template allowed for rapid improvements in GR activity resulting in potent, selective, nonsteroidal GR antagonists, CP-394531 and CP-409069.

RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:330268 CAPLUS

DN 136:340682

TI Preparation of oxadiazolylalkoxyoctahydrophenanthrenes as glucocorticoid receptor modulators

IN Liu, Kevin Kun-Chin; Morgan, Bradley P.; Robinson, Ralph Pelton

PA Pfizer Products Inc., USA

SO Eur. Pat. Appl., 39 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	V111 1						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	EP 1201660	A1	20020502	EP 2001-308789	20011016		
	EP 1201660	B1	20050831				
	R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IT, LI, LU, NL,	SE, MC, PT,		
	IE, SI, LT,	LV, FI	, RO, MK,	CY, AL, TR			
	AT 303369	E	20050915	AT 2001-308789	20011016		
	ES 2246292	Т3	20060216	ES 2001-1308789	20011016		
	CA 2360313	AA	20020430	CA 2001-2360313	20011026		
	US 2004014741	A1	20040122	US 2001-12274	20011026		
	US 6852719	B2	20050208				
	JP 2002193955	A2	20020710	JP 2001-330283	20011029		
	BR 2001004834	Α	20020820	BR 2001-4834	20011029		
PRAI	US 2000-244302P	P	20001030				
os	MARPAT 136:340682						
GI							

$$R^2$$
 R^2
 R^1
 R^3
 R^3

AB Title compds. [I; R1 = alkyl, trifluoroalkyl, C.tplbond.CMe,
 C.tplbond.CCl, C.tplbond.CCF3, CF3, etc.; R2 = alkyl, alkenyl,
 (substituted) Ph; R3 = alkyl, amino, aminoalkyl, heterocyclyl,
 heterocyclylalkyl; Q = (CH2)n; n= 1-3; with provisos], were prepared for
 treatment of obesity, diabetes, inflammation, anxiety, depression, and
 neurodegeneration (no data). Thus, ethanimidamide, N-hydroxy-2 [[4b,5,6,7,8,8a,9,10-octahydro-7-hydroxy-4b-(phenylmethyl)-7 (trifluoromethyl)-2-phenanthrenyl]oxy]- (preparation given) and NaH in THF were
 heated at 60° for 20 min. The solution was cooled to room temperature and
 ethyl-N,N-dimethylglycine was added. The resultant mixture was heated to
 reflux for 1 h to give 57% 2-phenanthrenol, 7-[[5-[(dimethylamino)methyl] 1,2,4-oxadiazol-3-yl]methoxy]-1,2,3,4,4a,9,10,10a-octahydro-4a (phenylmethyl)-2-(trifluoromethyl)-, [2R-(2α,4aα,10aβ)].

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:330265 CAPLUS
- DN 136:340594
- Preparation of 4b(S)-benzyl-7(S)-hydroxy-7-(3,3,3-trifluoropropyl)-4b,5,6,7,8,8a(R),9,10-octahydrophenanthrene-2-carboxylic acid (2-methylpyridin-3-ylmethyl)amide via an amidation reaction using carbonyldiimidazole.
- IN Murry, Jerry Anthony; White, Timothy Donald
- PA Pfizer Products Inc., USA
- SO Eur. Pat. Appl., 53 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN. CNT 1

GI

FAN.	PATENT NO.		DATE	APPLICATION NO.			
PI	EP 1201655 EP 1201655 EP 1201655	A2 A3	20020626	EP 2001-309057	20011025		
	R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IT, LI, LU, NL, CY, AL, TR	SE, MC, PT,		
	US 2002087005 US 6570020	A1	20020704	US 2001-8619	20011022		
	CA 2360024	AA	20020427	CA 2001-2360024			
	CA 2539147 ZA 2001008797		20020427 20030425				
	AT 303992 ES 2246293		20050915 20060216	AT 2001-309057 ES 2001-1309057			
	AU 784269	B2	20060302	AU 2001-83622	20011025		
	CN 1356319 JP 2002193937		20020703	CN 2001-135596 JP 2001-329529			
	CN 1680243	· A	20051012	CN 2005-10004526	20011026		
	BR 2001004836 RU 2219170	A C2	20021015 20031220				
	US 2003120081 US 6727392	A1 B2	20030626 20040427	US 2002-271309	20021015		
PRAI	US 2000-243873P	P	20001027				
	US 2001-8619 CA 2001-2360024		20011022 20011025				
	CN 2001-135596	A3	20011026				
os	CASREACT 136:340594						

AB Title compound (I) was prepared via reaction of 4b(S)-Benzyl-7(S)-hydroxy-7-(3,3,3-trifluoropropyl)-4b,5,6,7,8,8a(R)-9,10-octahydrophenanthrene-2carboxylic acid (II) with 3-aminomethyl-2-methylpyridine (III) in the presence of carbonyldiimidazole. Thus, II (preparation given) and carbonyldiimidazole were refluxed 2 h in THF; III in THF was added followed by stirring for 3 h at room temperature to give 69% I.

L6 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

2002:330263 CAPLUS AN

DN 136:340495

ΤI Preparation of octahydrophenanthrenyl carbamates as glucocorticoid receptor modulators

IN Liu, Kevin Kun-Chin; Morgan, Bradley Paul; Robinson, Ralph Pelton, Jr.

PA Pfizer Products Inc., USA

SO Eur. Pat. Appl., 42 pp. CODEN: EPXXDW

Patent

DT LΑ English

FAN.	CNT I						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	EP 1201649	A1	20020502	EP 2001-309064	20011025		
	EP 1201649	В1	20060531				
	R: AT, BE, CH,	DE, DK	, ES, FR, GE	B, GR, IT, LI, LU, NL,	SE, MC, PT,		
	IE, SI, LT,		, RO, MK, CY				
	JP 2002193911	A2	20020710	JP 2001-328050	20011025		
	CA 2360308	AA	20020428	CA 2001-2360308	20011026		
	CA 2360308	С	20060207				
	US 2002107235	A1	20020808	US 2001-6215	20011026		
	BR 2001004831	A	20020820	BR 2001-4831	20011026		
PRAI	US 2000-243993P	P	20001028				
os	MARPAT 136:340495						
GI							

$$\mathbb{R}^{2}$$
 \mathbb{R}^{1}
 \mathbb{R}^{3}
 \mathbb{R}^{4}
 \mathbb{R}^{3}

Title compds. [I; R1 = (trifluoromethyl)alkyl, CF3, C.tplbond.CMe, AB C.tplbond.CCl, C.tplbond.CCF3, CH2OA; A = (trifluoromethyl)alkyl; R2 = alkyl, alkenyl, (substituted) Ph; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, haloalkynyl; R4 = H , alkylamino, alkylhet; R3R4N = het; het = (substituted) 5-7 membered (unsatd.) heterocyclic ring containing 1-3 of N, O, S; and including any bicyclic group in which any of the above heterocyclic rings is fused to a benzene ring or another heterocyclic ring; and optionally substituted with 1-4 R7; R7 = (substituted) alkyl; with provisos], were prepared for treatment of obesity, diabetes, depression, anxiety, neurodegeneration, and inflammatory disease (no data). A solution of 2,7-phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-4a-(phenylmethyl)-2ethyl-[2R-(2α , $4a\alpha$, $10a\beta$)] (preparation given), COC12, and Et3N in THF was stirred at room temperature for 3 h; 1-(2-aminoethyl)pyrrolidine was added followed by stirring overnight to give 41% carbamic acid, [2-(1-pyrrolidinyl)ethyl]-, (4bS,7R,8aR)-7-ethyl-4b,5,6,7,8,8a,9,10octahydro-7-hydroxy-4b-(phenylmethyl)-2-phenanthrenyl ester.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:86132 CAPLUS
- DN 136:332658
- TI Scandium ion-promoted photoinduced electron transfer oxidation of fullerenes by p-benzoquinones
- AU Fukuzumi, Shunichi; Mori, Hisahiro; Imahori, Hiroshi; Suenobu, Tomoyoshi; Araki, Yasuyuki; Ito, Osamu; Kadish, Karl M.
- CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, Japan Science and Technology Corporation (JST), Suita, 565-0871, Japan
- SO Proceedings Electrochemical Society (2001), 2001-11(Fullerenes--Volume 11: Fullerenes for the New Millennium), 27-40 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- AB In the presence of scandium triflate, an efficient photoinduced electron transfer from the triplet excited state of C60 to p-chloranil occurs to produce C60 radical cation which has a diagnostic NIR (near IR) absorption band at 980 nm. The observed second-order rate constant of electron transfer (ket) increases linearly with increasing scandium ion concentration In contrast

to the case of p-chloranil, the ket value for electron transfer from 3C60* to p-benzoquinone exhibits first-order dependence on [Sc3+] at low concns., changing to second-order dependence at high concns. Such a mixture of first-order and second-order dependence on [Sc3+] is also observed for a Sc3+-promoted electron transfer from CoTPP (TPP2- = tetraphenylporphyrin dianion) to p-benzoquinone. This is ascribed to formation of 1:1 and 1:2

complexes between semiquinone radical anion and Sc3+ at low and high concns. of Sc3+, resp., which results in acceleration of the rate of electron transfer. The Sc3+-promoted electron transfer rate consts. have been determined for photoinduced electron transfer from the triplet excited states of C60 derivs. as well as higher fullerenes and the values are compared with the ionization potentials of these fullerene derivs.

- RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:848926 CAPLUS
- DN 136:119162
- TI Preparation and characterization of a new solvent-free polymer electrolyte based on spiroketal structure
- AU Tsutsumi, Hiromori; Shirotani, Rumiko; Onimura, Kenjiro; Oishi, Tsutomu
- CS Department of Applied Chemistry and Chemical Engineering, Faculty of Engineering, Yamaguchi University, Yamaguchi, 755-8611, Japan
- SO Electrochemical and Solid-State Letters (2001), 4(12), A195-A196 CODEN: ESLEF6; ISSN: 1099-0062
- PB Electrochemical Society
- DT Journal
- LA English
- AB Solvent-free solid polymer electrolytes based on spiropolymers were prepared and their properties were confirmed by conductance, differential scanning calorimetry, and X-ray diffraction measurements. The spiropolymer was synthesized from the bicyclic diketone and pentaerythritol. The spiro-polyketal (SP) dissolves lithium perchlorate and the conductivity of the (SP)1.5(LiClO4)1 complex is 4.24 + 10-5 S cm-1 at 30° and 3.83 + 10-4 S cm-1 at 60°.
- RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:847183 CAPLUS
- DN 136:142421
- TI Scandium Ion-Promoted Photoinduced Electron-Transfer Oxidation of Fullerenes and Derivatives by p-Chloranil and p-Benzoquinone
- AU Fukuzumi, Shunichi; Mori, Hisahiro; Imahori, Hiroshi; Suenobu, Tomoyoshi; Araki, Yasuyuki; Ito, Osamu; Kadish, Karl M.
- CS Department of Material and Life Science Graduate School of Engineering, Osaka University CREST, Japan Science and Technology Corporation (JST), Suita, Osaka, 565-0871, Japan
- SO Journal of the American Chemical Society (2001), 123(50), 12458-12465 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- AB In the presence of scandium triflate, an efficient photoinduced electron transfer from the triplet excited state of C60 to p-chloranil occurs to produce C60 radical cation which has a diagnostic NIR (near-IR) absorption band at 980 nm, whereas no photoinduced electron transfer occurs from the triplet excited state of C60 (3C60*) to p-chloranil in the absence of scandium ion in benzonitrile. The electron-transfer rate obeys pseudo-first-order kinetics and the pseudo-first-order rate constant increases linearly with increasing p-chloranil concentration. The observed second-order rate constant of electron transfer (ket) increases linearly with increasing scandium ion concentration. In contrast to the case of the C60/p-chloranil/Sc3+ system, the ket value for electron transfer from

3C60* to p-benzoquinone increases with an increase in Sc3+ concentration ([Sc3+])

to exhibit a first-order dependence on [Sc3+], changing to a second-order dependence at the high concns. Such a mixture of first-order and second-order dependence on [Sc3+] is also observed for a Sc3+-promoted electron transfer from CoTPP (TPP2- = tetraphenylporphyrin dianion) to p-benzoquinone. This is ascribed to formation of 1:1 and 1:2 complexes between the generated semiquinone radical anion and Sc3+ at the low and high concns. of Sc3+, resp. The transient absorption spectra of the radical cations of various fullerene derivs. were detected by laser flash photolysis of the fullerene/p-chloranil/Sc3+ systems. The ESR spectra of the fullerene radical cations were also detected in frozen PhCN at 193 K under photoirradn. of the fullerene/p-chloranil/Sc3+ systems. The Sc3+-promoted electron-transfer rate consts. were determined for photoinduced electron transfer from the triplet excited states of C60, C70, and their derivs. to p-chloranil and the values are compared with the HOMO (HOMO) levels of the fullerenes and their derivs.

RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:338070 CAPLUS
- DN 134:336224
- TI Use of corticotropin releasing factor (CRF) antagonists for treating syndrome X
- IN Chen, Yuhpyng Liang; Hamanaka, Ernest Seiichi
- PA Pfizer Products Inc., USA
- SO Eur. Pat. Appl., 55 pp. CODEN: EPXXDW
- DT Patent
- LA English
- FAN.CNT 2

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	PA	CENT	NO.			KIND DATE				APPLICATION NO.						DATE			
PΙ	ΕP	1097	709			A2		2001	0509	EP	20	000-	3094	41		2	0001	026	
EP 1097709				A3 20051221															
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, G	R,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY, A	L								
	ΑU	7767	24			В2		2004	0916	AU	20	000-	6669	5		2	0001	024	
	zA	2000	0060	80		Α		2002	0426	ZA	. 20	000-	6008			2	0001	026	
	US	6589	947			В1		2003	0708	US	20	000-	6968	22		2	0001	026	
	CA	2325	069			AA		2001	0429	CA	. 20	000-2	2325	069		2	0001	027	
	ΝZ	5078	125			Α		2004	1126	NZ	20	000-	5078	25		2	0001	027 ′	
PRAI	US	1999	-162	340P		P		1999	1029						•				
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OS MARPAT 134:336224

- AB Compns. and methods are provided for achieving a therapeutic effect, including the treatment or prevention of syndrome X in an animal, preferably a mammal including a human subject or a companion animal, using a CRF antagonist alone or together with a glucocorticoid receptor antagonist.
- L6 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:136227 CAPLUS
- DN 134:340801
- TI Photochemical Generation of Polymeric Alkyl-C60 Radicals: ESR Detection and Identification
- AU Qu, Baojun; Hawthorn, Geoff; Mau, Albert W. H.; Dai, Liming
- CS State Key Laboratory of Fire Science and Department of Polymer Science and

- Engineering, University of Science and Technology of China, Hefei Anhui, 230026, Peop. Rep. China
- SO Journal of Physical Chemistry B (2001), 105(11), 2129-2134 CODEN: JPCBFK; ISSN: 1089-5647
- PB American Chemical Society
- DT Journal
- LA English
- ESR spectroscopy has been used to study various alkylfullerene radical AB adducts generated by UV-photoinitiated reactions between low-d. polyethylene (LDPE) and C60 in the presence or absence of benzophenone (BP) as a photoinitiator under different conditions. Photolysis of LDPE/BP/C60 mixture in toluene at 323 K produced benzylfullerene (RC60) radical adducts, showing a strong ESR signal of g = 2.00270 with several well-resolved pairs of 13C satellites. On the other hand, a well-resolved ESR spectrum characteristic of polymeric alkylfullerene (PC60) radical adducts was observed during UV irradiation of the LDPE/BP/C60 in benzene or in the molten state (413 K). Detailed analyses of hyperfine structures (hfs) revealed that the ESR spectrum for PC60 radical adducts consisted of three components: (1) a broad singlet at g = 2.002 50 arising from C60 radical anions; (2) an innermost pair of 13C satellites; and (3) a 12-line spectrum superimposed on the broad singlet. Spectroscopic simulation allowed the 12-line spectrum to be attributed to the coexistence of two polymeric radical adducts of C60 (i.e., the tertiary carbon radical adduct, - (CH2) 3C-C60•, designated as PAC60•, and the secondary carbon radical adduct, -(CH2)2CH-C60•, designated as PBC60•), which have slightly different g values (gA = 2.002 48 and gB = 2.002 44) and integral intensities IA/IB (48.4/51.6). These results clearly indicated the generation of C60-bonded LDPE materials simply by photoirradn. of LDPE/C60 with BP as a photoinitiator.
- RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:88082 CAPLUS
- DN 134:246396
- TI Effects of lowering symmetry on the ESR spectra of radical anions of fullerene derivatives
- AU Fukuzumi, Shunichi; Mori, Hisahiro; Suenobu, Tomoyoshi; Imahori, Hiroshi; Gao, Xiang; Kadish, Karl M.
- CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, JAPAN Science and Technology Corporation, Suita, 565-0871, Japan
- SO Proceedings Electrochemical Society (2000), 2000-10(Fullerenes 2000--Volume 8: Electrochemistry and Photochemistry), 18-30 CODEN: PESODO; ISSN: 0161-6374
- PB Electrochemical Society
- DT Journal
- LA English
- AB Radical anions of dibenzyl adducts of C60, 1,4-(C6H5CH2)2C60·- and 1,2-(C6H5CH2)2C60·-, give ESR spectra which have larger g values (2.0004 and 2.0001, resp.) and much smaller linewidths (ΔHmsl = 2.5 and 3.9 G, resp. at 213 K) than the g value (1.9984) and the ΔHmsl value (30.9 G at 213 K) of C60·-. An even smaller ΔHmsl value (0.17 G) and a larger g value (2.0011) are observed in the tetrabenzyl C60 adduct radical anion, 1,4,10,24-(C6H5CH2)4C60·-. This is ascribed to a large splitting of the degenerate tlu orbitals caused by introduction of four benzyl groups to C60. In this case, a hyperfine structure, due to two nonequivalent protons of only one benzyl group (aH1

= 0.31 G, aH2 = 0.11 G), is observed and this is consistent with the predicted localized spin d. at the C2 position next to the C1 carbon to which a benzyl group is attached. The radical anions of the mono- and bisadducts formed in the Diels-Alder cycloaddn. reaction of C60 with 9,10-dimethylanthracene show ESR signals at different g values (2.0003 for the monoadduct and 2.0009 for the bisadduct). The relation between lower symmetry and the ESR spectra of radical anions of various C60 derivs. is discussed based on the change in the g values and the linewidths. The energy gap (δ) between the singly occupied orbital and the two other orbitals which had the tlu symmetry prior to introduction of addends to C60 is derived from the difference in the g values of various C60-derivs. from the free spin value (2.0023). There is a linear correlation between log δ Hmsl and $-\delta$.

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:790448 CAPLUS
- DN 133:350060
- TI Preparation of nonracemic octahydrophenanthrene and other tricyclic derivs. as selective modulators of glucocorticoid receptors
- IN Dow, Robert Lee; Liu, Kevin Kun-Chin; Morgan, Bradley Paul; Swick, Andrew Gordon
- PA Pfizer Products Inc., USA
- SO PCT Int. Appl., 279 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN CNT 2

FAN.	CNT 2																
	PATENT	NO.			KIND DATE			APPLICATION NO.						DATE			
PI	WO 2000066522 A1				20001109 WO 2000-IB366					20000327							
	W:	ΑE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG	, BR,	BY,	CA,	CH,	CN,	CR,	CU,
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		MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT	, RO,	RU,	SD,	SE,	SG,	SI,	SK,
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							20001109 CA 2000-2372173 20020122 BR 2000-10138										
	EP 1175																
	R:							FR,	GB,	GR	, IT,	LI,	LU,	NL,	SĒ,	MC,	PT,
	mp 0001		•		LV,	•		0501			0001						
	TR 2001	10310	4 60		T2		2002	1017		TR	2001-	3104			21	0000.	32 /
	JP 2002																
	EE 2001 NZ 5144						2003) 2003:				2001-					0000:	
	AU 7766	:00			A		2003. 2004:				2000- 2000-						
	CN 1781						2004				2005-		-		_		
	US 6380				B1		2002				2000-					0000.	
	ZA 2001						2002				2001-						
	NO 2001				Α		2001				2001-						
	HR 2001		. —				2002				2001-						
	BG 1061										2001-						
	US 2002	1473	36		A 1						2002-					00202	
	US 6699				В2		2004										

	US 2003199527	A1	20031023	US 2003-413879	20030415
	US 6777404	B2	20040817		
	US 2004176595	A1	20040909	US 2003-721318	20031125
PRAI	US 1999-132130P	P	19990430		
	US 1999-162340P	P	19991029		
	CN 2000-806949	A3	20000327		
	WO 2000-IB366	W	20000327		
	US 2000-559384	A 3	20000427		
	US 2000-696822	A3	20001026		
	US 2002-80174	A1	20020219		
os	MARPAT 133:350060				
GI					

AB Title compds. [e.g., I; D = CR7, CR7R16, N, NR7, O' E = C, CR6, N; F =CR4, CR4R5, O; R = XR1; R1 = H, alkyl, acylalkyl, arylalkyl, etc.; R2 = H, halo, alkyl, alkoxy, etc.; R3 = H, alkyl, arylalkyl, etc.; 1 of R2,R3 = null when adjacent dashed line = bond; R4,R5 = H, cyano, alkyl, alkoxy, etc.; R4R5 = O; R6 = H, cyano, alkyl, alkoxy, OH, etc.; R7,R16 = H, halo, cyano, alkyl, etc.; R7R16 = O; R8R9 = atoms to complete a substituted heteroarom. ring; R14,R15 = H, halo, alkyl, alkoxy, etc.; R14R15 = O when adjacent dashed lines = null; X = bond, CH2, CH(OH), CO; Z = (un) substituted CH2, -CH2CH2, -CH2CO, CO, etc.; dashed lines = optional bonds] were prepared as glucocorticoid receptor modulators (no data). E.g., 6-methoxy-2-tetralone was alkylated by formation of the pyrrolidine enamine and alkylation with benzyl bromide; the benzylated ketone then undergoes asym. Michael addition with Me vinyl ketone in the presence of $(S)-(-)-\alpha$ -methylbenzylamine followed by cyclocondensation with sodium methoxide to give a nonracemic methoxytetrahydrophenanthrenone derivative E.g., demethylation of the methoxytetrahydrophenanthrenone with boron trichloride, reduction of the enone with lithium and ammonia, addition of 1-lithiopropyne to the ketone, formation of the aryl triflate with triflic anhydride and carbonylation with carbon monoxide in the presence in the presence of palladium acetate and bis(diphenylphosphino)propanol gives an

hydroxyoctahydrophenanthrenecarboxylic acid derivative which is coupled with 4-(aminomethyl)pyridine in the presence of trimethylaluminum to give the octahydrophenanthrenecarboxamide II as one of the title compds.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:745440 CAPLUS
- DN 134:29098
- TI Effects of Lowering Symmetry on the ESR Spectra of Radical Anions of Fullerene Derivatives and the Reduction Potentials
- AU Fukuzumi, Shunichi; Mori, Hisahiro; Suenobu, Tomoyoshi; Imahori, Hiroshi; Gao, Xiang; Kadish, Karl M.
- CS Department of Material and Life Science Graduate School of Engineering, Osaka University CREST Japan Science and Technology Corporation, Suita Osaka, 565-0871, Japan
- SO Journal of Physical Chemistry A (2000), 104(46), 10688-10694 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English
- Radical anions of dibenzyl adducts of C60, 1,4-(C6H5CH2)2C60- and AΒ 1,2-(C6H5CH2)2C60--, give ESR spectra which have larger q values (2.0004 and 2.0001, resp.) and much smaller line widths ($\Delta Hms1 = 2.5$ and 3.3 G, resp., at 213 K) than the g value (1.9984) and the $\Delta Hmsl$ value (30.9 G at 213 K) of C60•-. An even smaller ∆Hmsl value (0.17 G) and a larger g value (2.0011) are observed for the tetrabenzyl C60 adduct radical anion, 1,4,10,24-(C6H5CH2)4C60- and this is ascribed to a large splitting of the degenerate tlu orbitals caused by introduction of four benzyl groups to C60. In this case, a hyperfine structure, due to two nonequivalent protons of only one benzyl group (aH1 = 0.31 G, aH2 = 0.11 G), is observed and this is consistent with the predicted localized spin d. at the C2 position next to the C1 carbon to which a benzyl group is attached. The radical anions of the mono- and bisadducts formed in the Diels-Alder cycloaddn. reaction of C60 with 9,10-dimethylanthracene show ESR signals at different g values (2.0003 for the monoadduct and 2.0009 for the bisadduct). The relationship between lower symmetry and the ESR spectra of radical anions of various C60 derivs. is discussed in terms of the g values and the line widths. The energy gap (δ) between the singly occupied orbital and the two other orbitals which had a tlu symmetry prior to introduction of addends to C60 is derived from differences in the g values of various C60•- derivs. from the free spin value (2.0023). A linear correlation is shown to exist between log Δ Hmsl and $-\delta$. The δ values are also obtained from Arrhenius plots of $\ln \Delta Hmsl$ vs T-1 and they agree well with the values derived from the g values and the reduction potentials.
- RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:601308 CAPLUS
- DN 133:266381
- TI Photoalkylation of C60 by alkylcobalt(III) complexes
- AU Ohkubo, Kei; Fukuzumi, Shunichi
- CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, JAPAN Science and Technology Corporation, Suita, 565-0871, Japan
- SO Inorganic Reaction Mechanisms (Amsterdam) (2000), 2(1-2), 147-153

- CODEN: IRMEFE; ISSN: 1028-6624
- PB Gordon & Breach Science Publishers
- DT Journal
- LA English
- AB Photolysis of a benzonitrile solution of alkylcobalt(III) complexes, [RCo(DH)2py] (R = Me and PhCH2, (DH)2 = bis(dimethylglyoximato), py = pyridine) in the presence of C60 by using visible light results in alkylation of C60 to yield R2C60. The excited state of [RCo(DH)2py] rather than C60 is responsible for the photoalkylation of C60, since the action spectrum for formation of R2C60 agrees with the absorption spectrum of [RCo(DH)2py] which is quite different from that of C60. The photoalkylation of C60 is retarded by a radical trapping reagent such as 2,2,6,6-tetramethyl-1-piperidinyloxyl radical (TEMPO). This indicates that photoalkylation of C60 proceeds via photocleavage of the cobalt-carbon bond of [RCo(DH)2py]. The intermediate benzyl radical produced by the photocleavage reaction of [PhCH2Co(DH)2py] is detected by ESR.
- RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:359956 CAPLUS
- DN 133:135092
- TI Stepwise Synthesis of Fullerene Cyclopentadienide R5C60- and Indenide R3C60-. An Approach to Fully Unsymmetrically Substituted Derivatives
- AU Sawamura, Masaya; Toganoh, Motoki; Suzuki, Kazuhiro; Hirai, Atsushi; Iikura, Hitoshi; Nakamura, Eiichi
- CS Department of Chemistry, The University of Tokyo, Tokyo, 113-0033, Japan
- SO Organic Letters (2000), 2(13), 1919-1921 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 133:135092
- AB Fullerene cyclopentadienide (PhCH2)2Ph3C60- and indenide (PhCH2)2PhC60-, each bearing two different organic groups, were efficiently synthesized through regioselective reactions of 1,4-(PhCH2)2C60 with an organocopper reagent (PhMgBr/CuBr.SMe2) or a Grignard reagent (PhMgBr) followed by deprotonation with KOCMe3.
- RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:355978 CAPLUS
- DN 133:58486
- TI CIDEP Studies of Fullerene-Derived Radical Adducts
- AU Koptyug, Igor V.; Goloshevsky, Artem G.; Zavarine, Igor S.; Turro, Nicholas J.; Krusic, Paul J.
- CS International Tomography Center, Novosibirsk, Russia
- SO Journal of Physical Chemistry A (2000), 104(24), 5726-5731 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English
- AB Photolyses of solns. containing organomercury compds. (HgR2) in the presence of C60 fullerene have been investigated by Fourier transform time-resolved EPR (FT TR EPR) and continuous-wave EPR (CW EPR) techniques. By FT TR EPR, both electron-spin-polarized 3C60 (A polarization) and

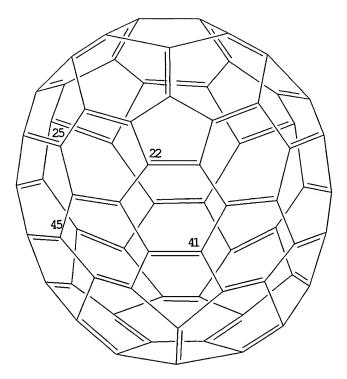
electron-spin-polarized adducts •C60R (E/A + E polarization) are observed The CW EPR spectra of the •C60R radicals under steady-state irradiation also exhibit some electron-spin polarization. The chemical induced dynamic electron polarization (CIDEP) in the FT TR EPR expts. is explained by the following series of steps. Photolysis initially causes cleavage of the organomercury compds. into radicals that add to C60 to form •C60R. The latter combine to form the dimers, [C60R]2, which are thermally stable and accumulate in the samples. In all of the reported expts., a certain quantity of dimers is produced by photolysis before the EPR spectra are acquired. In the FT TR EPR expts., laser excitation produces 3C60 by excitation of C60 and •C60R by photocleavage of the dimers. The observed E/A CIDEP patterns at short (<1 μ s) delays after the laser flash are proposed to be a result of the creation of polarization through the radical-pair mechanism (RPM) resulting from the interactions of two C60R radicals (geminate or free) formed from the photocleavage of [C60R]2 dimers. The addnl. E polarization observed at later times (>1 μ s) is proposed to result from the interaction of 3C60 with •C60R radicals, creating E polarization through the radical-pair-triplet mechanism (RPTM). The polarization observed in the CW EPR expts. is attributed to the maintenance of polarization through the radical lifetime because of the extremely long spin-lattice relaxation of the •C60R radicals. The latter conclusion is consistent with the very small (50 mG) line widths of the adduct radicals. An upper limit for the bond energy of the [C60R]2 dimers of 226 kJ/mol is established by the observation of the CIDEP of •C60R radicals when 532-nm excitation is employed. The role of multiple adducts in the observed FT TR EPR spectra is discussed.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:205506 CAPLUS
- DN 132:334150
- TI Effect of Addition Pattern on the Electrochemical and Spectroscopic Properties of Neutral and Reduced 1,2- and 1,4-(C6H5CH2)2C60 Isomers
- AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641,
- SO Journal of Physical Chemistry A (2000), 104(17), 3878-3883 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English
- AB The spectral and electrochem. properties of isomeric 1,2- and 1,4-adducts of fullerenes R2C60 were examined in their neutral, singly and/or doubly reduced forms. The 1st reduction potentials of 1,2- and 1,4-(C6H5CH2)2C60 in PhCN containing 0.1M TBAP are the same within exptl. error but the 2nd and 3rd redns. of the 2 isomers differ by 50 mV, with the 1,2-isomer being easier to reduce. Much larger differences, however, are seen in the near-IR spectra of the singly and doubly reduced organofullerene isomers. The monoanion of 1,2-R2C60 possesses an absorption band at .apprx.1000 nm, while the dianion has a band at .apprx.900 nm. The 1,4-R2C60 derivs. also show bands at similar wavelengths in their monoanionic and dianionic forms, but there is a 2nd near-IR band at 1500 (monoanion) or 1300 nm (dianion).
- RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:150054 CAPLUS
- DN 132:278876
- TI Splitting of Degenerate Orbitals of Dibenzyl and Tetrabenzyl Adducts of C60: ESR of the Radical Anions and the Rotation Barriers of Benzyl Groups
- AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Gao, Xiang; Kadish, Karl M.
- CS Department of Material and Life Science Graduate School of Engineering, CREST, Japan Sci. Technol. Corp., Osaka University, Suita, Osaka, 565-0871, Japan
- SO Journal of Physical Chemistry A (2000), 104(13), 2908-2913 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English
- AB The degenerate 2Elu ground state and the thermally accessible low-lying 2A2u excited state of C60•- give a broad ESR signal (ΔHmsl = 30.9 G at 213 K) which has a smaller g value (1.9984) as compared to the free spin value (2.0023) and linewidth which decreases with decreasing temperature (Δ Hms1 = 6.5 G at 133 K). The Ih symmetry of the parent C60 is lowered by the introduction of two benzyl groups to C60 to give 1,4-(C6H5CH2)2C60, which leads to the larger g value (2.0004) of 1,4-(C6H5CH2)2C60 - than that of C60 - (q = 1.9984) and a much smaller linewidth (\Delta Hmsl = 2.5 G at 213 K) which is independent of temperature An even smaller $\Delta Hmsl$ value (0.17 G) and a larger g value (2.0011) are observed in the tetrabenzyl C60 adduct radical anion, 1,4,10,24-(C6H5CH2)4C60•-. This is ascribed to a large splitting of the degenerate tlu orbitals caused by introduction of four benzyl groups to C60. In this case, a hyperfine structure due to two nonequivalent protons of only one benzyl group (aH1 = 0.31 G, aH2 = 0.11 G) is observed and this is consistent with the predicted localized spin d. at the C2 position next to the C1 carbon to which a benzyl group is attached. observation of two nonequivalent hyperfine coupling consts. due to the benzyl methylene protons indicates that rotation of the benzyl group at the Cl position is slow on the ESR time scale. The slow rotation rates of the benzyl groups in 1,4-dibenzyl adducts of C60 and the activation parameters were determined from a line broadening of the methylene protons in the 1H NMR spectra with increasing temperature
- RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:150053 CAPLUS
- DN 132:264799
- TI Electrogeneration and Characterization of (C6H5CH2)2C70
- AU Kadish, Karl M.; Gao, Xiang; Gorelik, Olga; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Journal of Physical Chemistry A (2000), 104(13), 2902-2907 CODEN: JPCAFH; ISSN: 1089-5639
- PB American Chemical Society
- DT Journal
- LA English

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AΒ (C6H5CH2)2C70 was electrosynthesized from C702- and C6H5CH2Br and purified by HPLC. Mass spectral results for the largest HPLC fraction confirm formation of the compound, while 1H NMR spectroscopy suggests that three isomers are present in this fraction, all of which are 1,4-addition products. The isomers are proposed to be the 22,25-, 22,41-, and 22,45-isomers (see locant labels on I) on the basis of 1H NMR data and the fact that bulky benzyl groups on C60 form preferentially 1,4- rather than 1,2-addition products. (C6H5CH2)2C70 was examined as to its electrochem. properties, and two sets of reduction processes were observed, one of which is assigned to the 22,25- and 22,41-isomers that exhibit identical electrochem. properties and the other to the 22,45-isomer of (C6H5CH2)2C70. The vis-near-IR spectrum of (C6H5CH2)2C70•- in benzonitrile shows a strong band at 776 nm which is not seen for C70 -- as well as two more bands in the near-IR region (1062 and 1250 nm) which are blue-shifted with respect to the near-IR absorption band of C70-- that appears at 1368 nm.

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- L6 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:22117 CAPLUS
- DN 132:222329
- TI Electrosynthesis and Structural Characterization of Two (C6H5CH2)4C60 Isomers
- AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi
- CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
- SO Journal of the American Chemical Society (2000), 122(4), 563-570 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal

LA English

AB The structural, spectral, and electrochem. properties of two (C6H5CH2)4C60 isomers are reported. One is designated as the 1,4;1,4-(C6H5CH2)4C60 isomer and the other as the 1,4;1,2-isomer of (C6H5CH2)4C60. The two isomers were isolated by HPLC from the products obtained by a reaction between [(C6H5CH2)2C60]2- and C6H5CH2Br. X-ray data show that the two (C6H5CH2)4C60 isomers differ from one another by the position of only one benzyl group and that, in each compound, the four benzyl addends are in close proximity. Both (C6H5CH2)4C60 isomers undergo three one-electron redns. in PhCN containing 0.1 M tetrabutylammonium perchlorate (TBAP) and have E1/2 values which are more neg. than values for either C60 or 1,4-(C6H5CH2)2C60. The mono-anions of 1,4;1,4- and 1,4;1,2-(C6H5CH2)4C60 were electrogenerated by bulk controlled-potential electrolysis in PhCN containing 0.2 M TBAP and characterized as to their spectral properties in both the visible and near-IR regions.

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